

Fragilisation des aciers de cuve irradiés : analyse numérique des mécanismes de plasticité à l'aide de simulations de dynamique des dislocations

Yang Li

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Dose-dependent embrittlement in nuclear reactor pressure vessel steel: dislocation-mediated plasticity mechanisms analyzed by means of 3D dislocation dynamics simulations

Thèse de doctorat de l'Université Paris-Saclay préparée à l'Ecole Normal Supérieure Paris-Saclay

Ecole doctorale n°579: Sciences mécaniques et énergétiques, matériaux et géosciences (SMEMAG) Spécialité de doctorat : Mécanique des solides

Thèse présentée et soutenue à Saclay, le 27 Septembre 2019, par

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ÉCOLE DOCTORALE

Sciences mécaniques et énergétiques, matériaux et géosciences (SMEMAG)

Titre : Fragilisation des aciers de cuve irradiés : analyse numérique des mécanismes de plasticité à l'aide de simulations de dynamique des dislocations

Mots clés : Dynamique des dislocations, Boucle prismatique, Effet d'irradiation

Résumé : Ce travail est une contribution à l'étude de la dégradation des propriétés mécaniques des matériaux métalliques irradiés, dans le contexte de la production d'énergie nucléaire. Cette thèse porte en particulier sur l'étude du comportement des dislocations dans les matériaux ferritiques irradiés, à l'aide de simulations de dynamigue des dislocations (DD).

L'évolution de la microstructure des défauts d'irradiation est tout d'abord analysée à l'aide d'un code nodal (code NUMODIS). Le Chapitre 2 traite en particulier de la diffusion et l'interaction de boucles prismatiques, en utilisant la dynamique des dislocations dite «stochastique». Ces calculs reproduisent les forces d'interaction élastiques boucle/boucle et les forces stochastiques associées aux fluctuations thermiques ambiantes. Il est ainsi montré que la réorientation des boucles (tilt) a un fort effet sur leur dynamique, en ce qui concerne notamment le taux d'évolution du confinement élastique boucle/boucle.

L'effet du glissement dévié sur l'interaction entre dislocation/boucle est ensuite examiné au Chapitre 3. Cette étude fait appel à une configuration initiale spécifique, associée à un changement du plan de glissement d'une source de dislocation

vis. De cette manière, il est montré que le glissement dévié réduit considérablement la résistance des défauts/obstacles. Cet effet confirme le rôle critique du glissement dévié durant la déformation plastique post-irradiation.

La déformation plastique post-irradiation est étudiée à l'échelle du grain, au Chapitre 4, à l'aide de simulations de DD à base de segments (code TRIDIS). Ces simulations traitent les mécanismes de glissement dévié et de glissement thermiquement activé (vis). Chaque condition d'irradiation simulée peut être caractérisée par un «décalage de la température apparente induite par des défauts d'irradiation \gg (Δ DIAT). Cette quantité est proportionnelle aux évolutions statistiques de la mobilité effective des dislocations. Le Δ DIAT calculé est pratiquement équivalent au décalage de la température de transition fragile à ductile ($\Delta DBTT$) obtenu expérimentalement, pour une taille et densité de défauts d'irradiation donnée. Cette corrélation $\Delta DIAT / \Delta DBTT$ peut être interprétée à partir de mécanismes de déformation plastique élémentaires, faisant appel à la théorie des dislocations.

Title : Dose-dependent embrittlement in nuclear reactor pressure vessel steel : dislocation-mediated plasticity mechanisms analyzed by means of 3D dislocation dynamics simulations

Keywords : Dislocation dynamics, Prismatic dislocation loop, Radiation effect

Abstract : The interplay between radiation-generated defects and dislocation networks leads to a variety of changes in mechanical properties and results in a detrimental effect on the structural reactor component lifetime. The present PhD work focuses on studying elementary and collective dislocation mechanisms in irradiated iron-based materials, by means of dislocation dynamics (DD) simulations.

Evolutions of the radiation-induced defect microstructure are studied first. Namely, the 1D diffusion of interacting prismatic loops is analyzed using the stochastic dislocation dynamics approach, accounting for the elastic forces acting between the loops and the stochastic forces associated with ambient thermal fluctuations. It is found that the interplay between stochastic forces and internal degrees of freedom of loops, in particular the loop reorientation, strongly influences the observed loop dynamics, especially the reaction rates resulting in the elastic confinement of loops.

The cross-slip effect on the dislocation/loop interactions is then examined using a specific initial confi-

guration associated with the glide plane change of a screw dislocation source, due to a single and well defined cross-slip event. It is shown that cross-slip significantly affects the effective strength of dislocation/defect interactions and therefore, post-irradiation plastic strain spreading.

Lastly, post-irradiation plastic strain spreading is investigated at the grain scale using segment-based dislocation dynamics simulations, accounting for the thermally activated (screw) dislocation slip and cross-slip mechanisms. It is shown that each simulated irradiation condition can be characterized by a specific "Defect-Induced Apparent Straining Temperature shift" (Δ DIAT) level, reflecting the statistical evolutions of the effective dislocation mobility. It is found that the calculated Δ DIAT level closely matches the ductile to brittle transition temperature shift (Δ DBTT) associated with the corresponding, experimentally-observed defect size and number density. This Δ DIAT/ Δ DBTT correlation can be explained based on plastic strain spreading arguments.

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Chapter 1

Applications of dislocation dynamics in irradiation scenarios

1 Industrial background

The safety and reliability of nuclear plants are inseparable from the performance of relevant materials used as structural components. Exposure to radiation conditions severely damages the microstructure of materials by displacing atoms from their lattice sites and generating additional helium and hydrogen impurities. The resulting microstructural evolutions then cause pronounced macroscopic mechanical property changes, including irradiation hardening, irradiation embrittlement and irradiation creep, that have detrimental effects on the performance and longevity of nuclear structural components (Bloom, 1998; Muroga et al., 2002; Chant and Murty, 2010; Zinkle and Was, 2013). A higher confidence in life-time assessments of these materials thus requires a detailed understanding of the related physical phenomena on a range of scales from the atomic level of single defects up to macroscopic effects.

The radiation effect on materials is a classic multiscale problem. Pertinent processes range from atoms to structural component length scales, spanning more than 10 orders of magnitude. Similarly, up to 22 orders of magnitude separate the characteristic time scale of atomic vibrations and the typical operation time of reactors (Odette et al., 2001; Cook, 2006). A large number of internal and external variables, including temperature, material microstructure, stress and irradiation conditions thus participate in this irradiation scenario.

Recent innovations in computational modeling, coupled with improved experimental techniques, provide a basis to develop validated multiscale models adapted to nuclear materials (Wirth et al., 2004; Samaras and Victoria, 2008; Malerba et al., 2008). Fig. 1.1 provides a schematic view of a multiscale approach integrating experimental and computational techniques to investigate materials degradation in the radiation environment. This approach implies information passing through different domains, each characterized by its specific experimental methods and simulation tools.

As the elementary radiation damage process is the displacement of atoms, molecular



FIGURE 1.1: Multiscale investigation of nuclear materials. (From Wirth et al. 2004)

dynamics (MD) simulations are widely used to study the radiation damage at the nanometric scale. Using this technique, it is well established that dense cascades in metals result in the production of both self-interstitial atom (SIA) clusters and vacancy clusters (De la Rubia et al., 1989; Marian et al., 2003; Bacon and Osetsky, 2004; Terentyev et al., 2008; Osetsky et al., 2005). The former can then evolve into prismatic dislocation loops subject to one-dimensional migration, while the latter evolves into various types ranging from stacking fault tetrahedra (SFTs), vacancy loops to large voids. In addition, the results from MD simulations have helped addressing a variety of dislocation/defect interaction mechanisms. However, the microstructural evolution and the mechanical change of irradiated materials are collective elasticity/plasticity phenomena that cannot be approached solely from an atomistic simulation point of view.

The other end of the multiscale investigation spectrum is represented by continuum solid mechanics. This framework takes particular advantages in solving rigorously the boundary value problem, namely, the conditions for mechanical equilibrium of a body submitted to internal and external applied fields. The most widespread computational technique is the finite element (FE) method. This calculation approach can easily address problems with length and time scales comparable to the experimental conditions (Odette et al., 2003; Dunne and Petrinic, 2005). Unfortunately, those gains are usually made at the expense of physical accuracy, and often requires incorporating inputs from small scale calculations to achieve the accuracy and consistency.

Dislocation dynamics (DD) has been developed for the purpose of bridging such micro and macro modelling approaches. It is a simulation technique that can capture both

long-range elastic interactions between dislocations and short-range interactions describing dislocation-defect interactions. DD simulations are therefore beneficial for studying the collective plasticity and the microstructural evolution at the material's grain scale. The simulation is especially applicable in cases where the plastic flow localization takes place. For example, experimental observations have clearly established the existence of a sharp and prominent yield drop both in irradiated face- and body-centered cubic (FCC, BCC) metals, associated with a highly heterogeneous plastic deformation mode and formations of "defect-depleted" dislocation channels (cf. Section 4.1). With the development of efficient algorithms, DD presents itself as the ideal technique to study these phenomena. The objective of Chapter 1 is to introduce the DD simulation technique, revisit its theoretical basis (see Section 2), and review some notable applications within the realm of irradiated materials (see Section 3 and 4).

2 Overview of DD method and its implementation

2.1 Initial developments

Two-Dimensional (in-plane) dislocation dynamics was first developed at the end of 1960s, for the sake of understanding the line tension and the equilibrium shape of dislocations under external stress (Brown, 1964). These early simulations yield valuable insight in modelling the activation of Frank-Read sources, the Orowan bypassing mechanism of precipitates and the hardening effect due to various types of obstacles (Foreman and Makin, 1966; Bacon et al., 1973). Another type of 2D simulations was developed later, wherein infinitely long dislocations of the same character pierce through the simulation plane that is viewed end-on (Lepinoux and Kubin, 1987; Ghoniem and Amodeo, 1988). However, these simulations were confined to planes either coinciding with the glide plane of the dislocation or parallel to the dislocation. The out-of-plane dislocation mechanisms such as climb, cross-slip and formation of junctions hence cannot be treated.

This 2D method was then extended to three dimensions by Amodeo and Ghoniem (1990) and Kubin et al. (1992), aiming at obtaining a more realistic description of individual and collective dislocation behaviours. 3D DD simulations were further developed (Zbib et al., 1998; Ghoniem and Sun, 1999; Schwarz, 1999; Shenoy et al., 2000; Weygand et al., 2001), separating into two major classes : the segment-based DD and the node-based DD. Within segment-based DD framework, a dislocation network is composed of piecewise linear segments. And the dynamic of dislocations is obtained through the evolution of a predetermined set of dislocation segments. This pre-defined set of segments contributes to minimizing the computational load on the elastic stress field. Therefore the segment-based DD is appropriate to study the collective behaviour of dislocations at length-scales up to microns. On the other hand, in node-based models, a dislocation line of arbitrary character is parameterized into a collection of nodes and the dynamic laws are directly applied to the nodes. This type of models thus performs a more accurate description on dislocation topology but is computationally more intensive compared to the

segment-based DD. The node based DD is usually adopted in studying the complex topological changes involving the multiple junction formation and the dislocation splitting. The rest of the section addresses these dislocation dynamics models in more detail.

2.2 General DD theory

Dislocation dynamics enables the computation of macroscopic properties directly from the evolution of the dislocation microstructure. In contrast to the atomistic methods where the degrees of freedom of the system depend on individual atoms, in DD, dislocations are treated as line defects responding to external stress and themselves act as source of stresses. The dynamics of dislocations is therefore affected by the stress fields coming from the dislocation network, the external stress applied on the simulation cell, the local stress due to the presence of the defects such as voids and precipitates (especially in irradiated materials).

The dislocation stress is usually computed from the static elastic theory. For instance, in a homogeneous infinite linear elastic solid, the stress field at position x generated from a closed dislocation loop C can be obtained from its contour integral (Mura, 1987; Anderson et al., 2017):

$$\underline{\underline{\sigma}}^{\infty}(\boldsymbol{x}) = \frac{\mu}{4\pi} \oint_{C} \left[(\boldsymbol{b} \times \nabla') \frac{1}{R} \otimes d\boldsymbol{l}' + d\boldsymbol{l}' \otimes (\boldsymbol{b} \times \nabla') \frac{1}{R} \right] - \frac{\mu}{4\pi(1-\nu)} \oint_{C} \nabla' \cdot (\boldsymbol{b} \times d\boldsymbol{l}') (\nabla \otimes \nabla - \underline{\underline{l}} \nabla^{2}) R$$
(1.1)

where $\nabla' = \partial/\partial x'_i$, R = ||x - x'|| and \underline{I} is the unit dyadic. Quantity b is the Burgers vector, μ is the shear modulus and ν is the Poisson ratio. Note that the stress field given by expression 1.1 is singular when the point x approaches the source point x' (i.e., R = 0) and therefore the use of regularization methods can be necessary (Cai et al., 2006; Arsenlis et al., 2007; Po et al., 2014a).

The objective of a DD simulation is to gain the dislocation configuration evolutions with time. Once obtaining the stress $\underline{\sigma}$ acting on the dislocations and assuming that dislocation motion is overdamped (Bulatov and Cai, 2006), it is possible to develop a dislocation mobility law $v(\underline{\sigma}, \boldsymbol{\xi}, \boldsymbol{b}, \boldsymbol{n}, T)$ based on local quantities including the line orientation $\boldsymbol{\xi}$, Burgers vector \boldsymbol{b} , slip plane normal \boldsymbol{n} and temperature T. Such line-object potentially contains an infinite number of degrees of freedom, however. A discretization procedure with conserved Burgers vector is hence required for numerical calculations. An arbitrary dislocation can be discretized into *nodes*, and inner-connected by *segments* as briefly discussed in Section 2.1. We will distinguish these different discretization methods and implementation strategies in the following section.

2.3 Different types of DD models

Segment-based DD. In this model, the dislocation is discretized into a series of pre-defined segments, including edge, screw and junctions orientations (Verdier et al., 1998; Devincre

et al., 2011). These dislocation segments are characterized by their length, center, line direction, Burgers vector, glide direction and etc. The calculation of the net stress acting on each segment is then typically performed in the segment midpoint. That net stress is the sum of the external stress and the internal stress due to other dislocations according to a given analytical expression (Devincre, 1995). Moreover, it is known that in absence of the applied stress, a curved dislocation tends to straighten out for the sake of minimizing its line length and strain energy. To account for this effect into the segment discretization scheme and also to avoid the divergence when calculating the self-stress (e.g., R = 0 in Eq. (1.1)), various corrective methods are implemented into DD codes, for instance introducing a line tension stress term τ_{lt} (Foreman, 1967),

$$\tau_{lt} = \frac{\mu b}{4\pi(1-\nu)R} (1-2\nu+3\nu\cos^2\theta) \left(\ln\frac{L}{2b} - \nu\cos2\theta\right)$$
(1.2)

where μ and v stand for the shear modulus and the Poisson ratio respectively. R is the radius of curvature, L is the dislocation length and θ is the angle between the Burgers vector and the line direction.

The total midpoint stress is then used to compute the segment velocity based on material-specific dislocation mobility law. For FCC type materials, it is usually assumed that the velocity v and the effective resolved shear stress τ^* obey a linear relation, such as:

$$v = \frac{\tau^* b}{B} \tag{1.3}$$

where *B* is the material and temperature dependent viscous coefficient. Although the lattice resistance in BCC metals is sometimes modelled using Eq. (1.3), the actual screw dislocation motion is, in general, thermal activated (Seeger, 1984; Kocks, 1975). Atomistic simulations always provide an accurate way to determine the dislocation mobility rule (Duesbery, 1983; Moriarty et al., 2002). Phenomenological mobility rules are nonetheless necessary in order to gain a complementary, coarse-grained (mesoscale) description of dislocation motion. For example, the screw dislocation velocity based on the kink-pair mechanism, is usually treated using an Arrhenius-like description (Tang et al., 1998):

$$v = AL \exp\left(-\frac{\Delta H(\tau^*)}{k_B T}\right)$$
(1.4)

where A is a coefficient depending on the critical kink-pair length, the Debye frequency and etc. L is the length of screw segment and $\Delta H(\tau^*)$ is the stress-dependent activation enthalpy.

The obtained midpoint velocity is then used to calculate the displacement of each segment, and the dislocation configuration is updated at each time step taking advantages of the discrete set of segment orientations (see Fig. 1.2a).

Node-based DD. The basis of the nodal DD formalism is the equation describing the force equilibrium condition for an elementary dislocation segment (Arsenlis et al., 2007; Drouet

et al., 2014). Assuming that the lattice drag force is proportional to the velocity v, this is:

$$\underline{B}\boldsymbol{v} = \boldsymbol{f}^{PK} \tag{1.5}$$

where $\underline{\underline{B}}$ is the drag coefficient (tensor), depending on the slip system and the straining temperature. The term f^{PK} is the driving force (or Peach-Koehler force) exerted by the stress field $\underline{\underline{\sigma}}$ where $f^{PK} = (\underline{\underline{\sigma}} \cdot \underline{b}) \times \boldsymbol{\xi}$. It is worth noting that in the nodal DD framework, the internal stress associated with dislocation networks is usually computed using the non-singular self-consistent stress formalism. This approach inherently account for the dislocation elastic interaction with itself (self-stress contribution) and hence, there is no need for the total stress field corrections such as the line tension term.

The dynamic variables in nodal DD simulations are the so-called nodes. The dislocation segments merely connect the node pairs as shown in Fig. 1.2b. The nodal velocities are then obtained by assembling and solving Eq. (1.5) using discrete numerical methods.

Another DD framework is called parametric DD (Ghoniem et al., 2000; Po et al., 2014b). This approach derives from the traditional node-based DD, which discretizes dislocations into a succession of splines rather than straight segments (see Fig. 1.2c). This type of DD utilizes the Galerkin finite element method to compute the nodal velocities, which thus allows an incorporation of nonlinear mobility laws and can then be applied to study the dislocation response due to non-Schmid effects.

2.4 Boundary conditions and optimization methods

Periodic boundary conditions. Periodic boundary conditions (PBC) are commonly used in 3D DD simulations for the sake of investigating representative volume elements embedded into large single crystals (Fivel and Canova, 1999; Cai et al., 2003). The entire system is therefore composed by a primary simulation cell accompanied by its multiple images. Each time a dislocation segment goes across a boundary, an image segment re-enters the opposite boundary at an equivalent position. In this case, geometrically necessary dislocations may generate cell curvatures that are incompatible with the transnational periodicity (Bulatov et al., 2000). The initial configuration indeed requires a net zero integral of the Nye's tensor over the whole primary cell. A general solution for this issue is to use the configurations with equilibrated Burgers vectors such as closed loops and infinite dipoles. Periodic boundary conditions induce additional artifact, called the self-annihilation of the dislocation lines. Various methods are available in literature, which help mitigating the influence of this effect, for instance, by setting the critical value of the self-annihilation distances and modifying the shape of the simulation cell into mutually incommensurate sizes (Madec et al., 2004).

Finite boundary conditions. The stress field computed from Eq. (1.1) is generally applied to an infinite medium. In the case of a finite volume however, internal stress field corrections are necessary, according to the mechanical boundary conditions utilized at the external surfaces. A method based on the superposition principle was proposed and applied in many of 3D DD simulation cases (Van der Giessen and Needleman, 1995; Fivel



FIGURE 1.2: Different dislocation discretization methods of (a) segment, (b) nodal and (c) parametric DD simulations. (From Marian et al. 2018)

and El-Azab, 1999; Weygand et al., 2002; Tang et al., 2006). Fig. 1.3 shows a typical finite simulation volume under boundary conditions with a displacement U^{app} on the portion of the surface $d_1\Omega$ and simultaneously an applied force F^{app} on $d_2\Omega$. It is seen that the effective stress $\sigma(M)$ inside such volume with the presence of dislocations is therefore the sum of two stresses, $\sigma_1(M)$ and $\sigma_2(M)$. $\sigma_1(M)$ is the stress field generated from dislocations in an infinite medium, which in turn result in force F^D and displacement U^D on $d_2\Omega$ and $d_1\Omega$, respectively. Term $\sigma_2(M)$ is the stress acting at the point M in a finite dislocation-free volume for given boundary conditions $F^{app} - F^D$ and $U^{app} - U^D$. The second problem can then be solved using various methods including finite element analysis.

Computational optimization. In molecular dynamic simulations, the total number of degrees of freedom (i.e., the number of atoms) is usually constant along with the simulation time. In DD simulations however, the number of dislocation segments may significantly increase up to a relatively large value due to dislocation multiplication and interactions, especially in large-scale simulations. This leads to an increase in computational cost, due to long-range dislocation interactions and therefore demands adaptive computational optimization methods to speed up the simulation. Specific methods have been developed in an attempt to deal with the segment-pair interactions. For instance, the fast multiple method (FMM) can reduce the asymptotic scaling of such calculation of a *N*-segment



FIGURE 1.3: Sketch of the superposition method applied to stress calculation in finite sized simulation space.

system from $O(N^2)$ to $O(N \log N)$ or even O(N) (Greengard and Rokhlin, 1987; Wang et al., 2004; Shin et al., 2006). The general idea is dividing the calculation of the dislocation interactions into long-range and short-range categories. The latter are computed explicitly at each time step with the near-by dislocation segments. The former contribution is considered to evolve slowly in time and space, and hence is computed every *n* time steps. Another similar method is developed and known as the under-integration (Weygand et al., 2009). That approach distinguishes between the slow and fast-evolving dislocation events, and therefore the former event can be updated in a larger time step compared to the latter one. It is especially useful in situations where a large fraction of the dislocations is immobilized at strong obstacles, including forest obstacles or grain boundaries. More recently, an enhanced subcycling time-integrators have been developed and implemented (Bertin et al., 2019). Likewise, this method works on isolating fast, ill-behaving modes from the rest of the system and integrate them separately, with the aid of GPU computation. Such GPU-implementation allows to circumvent the loss of scalability in parallel computations and therefore obtains large computational gains.

2.5 Local rules

In above section, we have briefly discussed how DD simulation works incorporating with different boundary conditions. The implementation of local rules enables DD to achieve a physically-based description of dislocation response to external loadings. This section addresses dislocation cross-slip, junction reactions and dislocation/defect interactions taking place in irradiated materials.

Cross-slip. Cross-slip is a phenomenon where screw dislocation segments change their glide plane. It is one of the most important annihilation, multiplication and obstacle bypassing mechanisms for gliding dislocations. For FCC metals, one well-known mechanism of cross-slips involves the recombination of the Shockley partial dislocations. The implication of this local rule in DD simulation was originally inspired by the Fridel-Escaig model (Bonneville et al., 1988; Kubin et al., 1992), taking the form of an activation probability written as:

$$P(l) = \beta \frac{l}{l_0} \frac{\Delta t}{t_0} \exp\left(\frac{-\Delta H_0}{k_B T}\right) \exp\left(\frac{\tau^* - \tau_{III}}{k_B T}V\right)$$
(1.6)

where β is a constant, l is the length of the considered screw segment, Δt is the discrete time step, l_0 and t_0 are referent length and time respectively. Term ΔH_0 is the activation energy, T is the temperature, V is the activation volume, τ^* is the resolved shear stress exerted on the segment and τ_{III} is the resolved shear stress at the onset of stage III of plastic deformation. This expression, used in combination with an usual Monte Carlo scheme, allows characterizing dislocation interactions involving cross-slip, including dipole annihilation and double cross-slip events (Robertson et al., 2001; Wang et al., 2007).

For BCC metals however, there is no well established cross slip rule yet. Screw dislocation cross-slip in BCC materials is intimately related with the straining temperature. At relatively high temperature (above the transition temperature), it is possible to use the same strategy as that for FCC metals, or even directly assigned with pencil glide. At low temperature however, screw dislocation motion is characterized by glide jump between two {110} planes sharing the same Burgers vector. The jump probability depends on the kink-pair activation energies in the two {110} involved planes. Cross-slip is favorable or not, according to the dislocation core configuration affected by the twinning-anti-twinning asymmetry of BCC crystals (Duesbery and Vitek, 1998; Marian et al., 2004; Chaussidon et al., 2006). At medium temperatures, slip traces tend to follow the maximum resolved shear stress (MRSS) plane. Non-Schmid effects thus weaken with the increase in the straining temperature (Taylor and Elam, 1926; Caillard, 2011).

Another phenomenon associated with the dislocation motion direction change is the dislocation climb. This will be discussed in Section 4.3.

Junction formation and destruction. Collision between a pair of attractive dislocation segments with Burgers vectors b_1 and b_2 may lead to the formation of junctions, for the sake of minimizing their total energy. The new segment thus has Burgers vector $b_3 = b_1 + b_2$, and the plausibility of such reaction is generally discussed in terms of the Frank's rule, which is energetically favorable if $b_3^2 < b_1^2 + b_2^2$. The destruction of such junction requires a critical stress to unzip the junction segment and retrieve the loss of the total energy. The validity of DD simulations is therefore usually checked by matching the critical stress of Lomer-Cottrell (LC) locks between atomistic and mesoscale simulations carried out using identical configurations.

Dislocation/defect interactions. It is of particular interest in developing a multiscale modelling framework applied to irradiated materials. This challenge entails treating a large

number/rate of small-scale interactions. Irradiation of metals induced various types of defects, including self-interstitial atoms (SIAs), vacancies, dislocation loops, vacancy loops, stacking fault tetrahedra (SFTs), voids, precipitates and others, which then strongly interact with mobile dislocations. In general, DD simulation of these interactions is inspired by other models, including MD and kinetic Monte Carlo (KMC) simulations. For instance, KMC scheme can provide useful information of dislocation motion in the presence of point defects like solutes, SIAs and vacancies. Coupled to DD simulations, it therefore enables the investigation of the effect of these defects on the post-irradiation deformation (Deo et al., 2005; Chen et al., 2008). As regards reactions between dislocations and other defects, the interaction mechanism and the corresponding defect strength are usually obtained by means of MD simulations (De la Rubia et al., 2000; Osetsky and Bacon, 2003). There are also many other models, which were developed over the years for treating various reactions between dislocations and defects (Rong et al., 2005; Sobie et al., 2015). In the next section, we will discuss these strategies and applications in detail.

3 Small-scale DD simulations and radiation-induced defects

Radiation-generated defect clusters interact with gliding dislocations as discussed in the previous section. The corresponding interaction mechanism depends on the defect (and dislocation) type, according to atomic scale MD simulations (please review articles of Bacon and Osetsky 2005 and Bacon et al. 2009). MD cannot be extended to all the interaction cases involving many-body effects, low stress rates or large size and time scales. Under such circumstance, DD is a possible alternative method for studying the post-irradiation deformation, where the small scale dislocation/defect interactions need to be implemented and cross-checked. In this section, we thus review some of the most important examples.

3.1 Dislocation loops

SIA clusters evolving in the form of the dislocation loop are typically observed in irradiated metals. It is characterized by its size, shape, line orientation and Burgers vector. The dislocation/loop reaction strongly depends on the local elastic interactions. DD simulations can therefore naturally capture the reaction detail and allow a direct treatment on elastic calculations. For example, Shi et al. (2015) have systematically studied reactions between a $1/2 \langle 111 \rangle \{110\}$ edge dislocation and a square-shaped $\langle 100 \rangle$ interstitial loop in α -Fe. These simulations have been validated by comparisons with corresponding MD results (Terentyev et al., 2008). One such reaction path is shown in Fig. 1.4. It is seen that in both DD and MD simulations, the loop is absorbed by the mobile edge dislocation in the form of a double superjog. The quantitative difference for the unpinning stress of the two methods is within 18%. DD simulations can therefore qualitatively and quantitatively reproduce dislocation/loop interactions by carefully identifying the dislocation mobility



FIGURE 1.4: Example of the interaction mechanism from MD and DD simulations between a $1/2 \langle 111 \rangle \{110\}$ edge dislocation and a square-shaped $\langle 100 \rangle$ interstitial loop in α -Fe. (From Shi et al. 2015)

as given in Eq. (1.4). Similar comparisons have been reported by Cui et al. (2017) and Li et al. (2018). They investigated the interactions between a $1/2\langle 111\rangle \{110\}$ screw dislocation and a hexagonal $\langle 111\rangle$ interstitial loop, and then compared to the MD results of Liu and Biner (2008).

Large-scale DD simulations, which considered dispersed loops with two types of Burgers vectors (100) and (111), have been widely studied in past years (Arsenlis et al., 2012; Gururaj et al., 2015a; Cui et al., 2017). These models do not require any particular assumptions and therefore are well-suited to describe the collective behaviour of dislocations in irradiated materials. The simulations bear the computational cost of the numerous elastic interactions due to the discrete representation of the loops. This difficulty can be addressed by treating the local interaction using several acceleration methods. For example, Cui et al. (2018c) have developed a DD method coupled with a continuum irradiation defect field. In their massive simulations, the defect field is considered as continuous and its density evolves according to a conservation equation. Gururaj et al. (2015b) have introduced one type of facet, in the form of planar, square-shaped surfaces representing an actual dislocation loop. These facets act as soft obstacles: gliding dislocations can cut through a given facet only if a local stress criterion is satisfied, depending on the mobile dislocation characters. The corresponding obstacle strength is usually calibrated based on MD simulation results. One example of such simplified reaction paths is shown in Fig. 1.5 for both edge and screw dislocation cases. In many important cases, the facet representation can correctly reproduce the interaction without any significant loss in accuracy, which is therefore beneficial for performing large-scale simulations (Gururaj et al., 2015a,b; Li and Robertson, 2018).

Plastic strain spreading at the grain scale usually takes the form of wavy shear bands, involving the ubiquitous cross-slip mechanism, e.g. as observed in iron by Obrtlik et al. (2005) and Robertson et al. (2007). Recently, Li et al. (2018, 2019c) and Gururaj (2013)



FIGURE 1.5: Example of the simplified reaction paths between a $1/2\langle 111\rangle \{110\}$ dislocation and two $\langle 100 \rangle$ oriented facets. (a) Edge dislocation case. (b) Screw dislocation case. (From Gururaj et al. 2015b)

have studied the cross-slip effect on such interactions, by constituting a specific initial configuration, associated with a screw dislocation glide plane change or a dissociation of a screw segment into partials in the cross-slip plane (only for FCC materials), due to a single and well defined cross-slip event. The results revealed that a dislocation encountering an obstacle along the gliding path can bypass it in the cross-slip plane, thus significantly reducing the effective interaction strength. Accordingly, it is concluded that the cross-slip mechanism is of particular importance in the grain scale post-irradiation plastic strain spreading. Similar results have been reported by Shin et al. (2003), who considered the interactions between a dislocation and precipitates in presence of the cross-slip (see details in Section 3.2).

3.2 Stacking fault tetrahedra, voids and precipitates

Stacking fault tetrahedra (SFTs) is another common radiation defect in FCC metals. Collisions between gliding dislocations and SFTs involve partial dislocation reactions that are difficult to deal with DD modelling. Progress in implementing partial dislocation models into DD frameworks has been recently achieved by Shenoy et al. (2000), Martinez et al. (2008b), and Marian et al. (2009), including implementations of an additional vector conservation rule of the dislocation splitting and a force acting on partial dislocations. These models thus enable the investigation of dislocation-SFT interactions in a physical way. For example, Martinez et al. (2008a,c) presented step-by-step DD reaction paths, and their comparison with the corresponding atomistic simulations, providing a more efficient insight in the interaction dynamic at a relatively low strain rate. More importantly, it was found that the strength of SFT directly depends on the intersection area of the dislocation glide plane and the SFT. Unfortunately, the time step used in their work dropped to a very small value that precluded the direct use of this into large scale DD simulations.

Voids and precipitates in irradiated metals impede the gliding of dislocations as well. A number of studies of the interaction between dislocations and precipitates/voids have been carried out by means of MD, which provided insight into dislocation bypass mechanisms at the atomic scale (please refer to reviews of Osetsky and Bacon 2003, 2010). For instance, it was found that small coherent precipitates can be sheared-off by moving dislocations, while large precipitates and voids may be regarded as impenetrable inclusions to dislocations. Dislocations overcome such strong obstacles by glide, dislocation climb, cross-slip and phase change. Moreover, the obstacle strength of voids and large precipitates obtained from MD is in general compatible with the prediction of the Bacon-Kocks-Scattergood (BKS) strengthening model. The latter is developed based on Orowan's interaction scheme and incorporates dislocation self-interactions, which gives the obstacle strength τ_c as (Bacon et al., 1973):

$$\tau_c = \frac{\mu b}{2\pi L} \left[\ln\left(\frac{\overline{D}}{b}\right) + \Delta \right]$$
(1.7)

where $\overline{D} = (D^{-1} + L^{-1})^{-1}$, *D* is the obstacle diameter, *L* is the obstacle spacing and Δ is an obstacle-specific fitting constant. It is worth noting that this model is inaccurate when the reaction implicates in partial dislocations for FCC metals especially if their separation is larger than the void size, or screw dislocations for BCC metals due to their thermal activated motion (Monnet et al., 2010; Lehtinen et al., 2018). In addition, this model includes many significant simplifications, which may result in other deviations. The foremost one is that the image forces due to the obstacles are only considered at the dislocation-surface intersection point and are neglected elsewhere (Crone et al., 2015).

Dislocation interactions with voids and precipitates affected by the image forces as well. These forces can be evaluated using the superposition principle, as explained in Section 2.4. The only difference is that, this time, an additional medium is present inside the simulation cell. This condition usually requires a correction stress $\sigma_{correct}$ to compensate for the stress field generated in the volume due to the inclusion. Crone et al. (2015)

considered the simulation of an edge dislocation encountering an array of voids using such finite-element-based DD method (see Fig. 1.6a), and then compared their void strength to the prediction from BKS model. It was found that the attractive image forces between the dislocation and free surface significantly reduce the obstacle strength of voids. In the case of precipitates, DD simulations carried out by Shin et al. (2003) have shown that the dislocation behaviour predicted by DD simulations is consistent with MD results when taking the image forces into account. More interestingly, they have found that dislocations can bypass precipitates by cross-slip (see Fig. 1.6b) and the image stress field around the inclusion seems to enhance the cross-slip probability throughout the interaction time.

In large scale calculations however, accurate image forces calculations for every obstacle comes at a significantly high computational cost. Phenomenological interaction laws informed by the aforementioned small scale simulations are once again more feasible. For example, Queyreau et al. (2011) have investigated the dislocation behaviour in presence of void ensembles in α -iron. Voids were assumed to be shearable particles whose resistance and thermal activation parameters were obtained from atomistic calculations. On the other hand, voids and precipitates can be treated as impenetrable particles. A variety of techniques to account for their strengthening effect in large-scale DD simulations have been proposed, generally inspired from MD results, experimental observations and other analytical models (Queyreau et al., 2010; Monnet et al., 2011; Ringdalen et al., 2017).

3.3 Stochastic DD

Based on above discussions, it is claimed that the DD scheme is an efficient technique for modelling various dislocation/obstacle interactions. In those cases, obstacles can be overcome only if the local applied stress on the dislocation is larger than an obstacle strength and the thermal activation is relatively weak, with respect to the corresponding mechanical work. Thermal activation process plays a crucial role for several cases however, e.g., when dislocations interact with weak or highly mobile obstacles under low strain rate loading, which is a common case in the deformation stage I of power law creep. Conventional deterministic DD models are therefore not applicable to such problems. Under this circumstance, Rönnpagel et al. (1993) devised a dislocation glide model, wherein the Langevin force associated with thermal fluctuations contributed to the dislocation motion. Their simulation thus successfully reproduced the jerky dislocation motion throughout an array of interacting obstacles. To extent this model to more general situations, Hiratani and Zbib (2002, 2003) developed a so-called stochastic dislocation dynamics (SDD), which enables modelling the three-dimensional dislocation behaviour by adding a random stress impulse in heuristic way to the equation of dislocation motion. The stochastic stress was assumed to be independent of the dislocation segment positions and its strength was taken in the form of a Langevin force. Using this SDD model, they have investigated the dislocation motion through periodically dispersed SFEs arrays, and examined a transient regime of obstacle-controlled dislocation motion and latticecontrolled dislocation motion in copper. In addition, the formation of dislocation patterns and the interaction of threading dislocations with immobile dislocation loops were fur-



b) Dislocation-precipitate interaction

FIGURE 1.6: DD simulation examples of the dislocation/obstacle interaction. (a) Left: Schematic of the DD simulation model for aluminum. The dotted lines are virtual segments to ensure the conservation of Burgers vectors. Right: Comparison of void strengths from different methods as a function of the harmonic average between void size and spacing. (From Crone et al. 2015) (b) Left: 3D simulation cell for copper. Right: Bypassing the precipitates by double cross-slip of a scrw dislocation. (From Shin et al. 2003)

ther studied using SDD and compared to a statistical analysis based on the Friedel-Kocks model. It was found that non-trivial fractal instability of the plastic strain could be correctly predicted by SDD simulations, when thermal and strain fluctuations are taken into account.

Recent progress on SDD models has been presented in the work of Li et al. (2019a). It



FIGURE 1.7: Snapshots from a stochastic dislocation dynamics simulation of a hexagonal initially pure prismatic loop at 100K.

showed the one-dimensional diffusion of prismatic loops in α -iron, using the discrete dislocation dynamics approach that explicitly includes the stochastic forces associated with ambient thermal fluctuations. The adopted stochastic force formalism was directly derived from the collective motion of the entire prismatic loop. Fig. 1.7 shows snapshots from a SDD simulation of a hexagonal prismatic loop. It is seen that the loop initially locates at the energetic saddle point where the loop Burgers vector is normal to its habit plane. Then, within a few picoseconds, the loop habit plane becomes tilted until reaching the local minimum depending on the temperature. For the loop-pair cases, three fundamental types of reactions have been observed and emulated: coalescence, repulsion, and confinement by elastic forces. It was found that the interplay between stochastic thermal forces and internal degrees of freedom of loops, in particular the reorientation of the loop habit planes, strongly influences the observed loop dynamics, especially for the confinement reactions, in terms of the bound state lifetime. This work thus suggests that it is important to include internal degrees of freedom of loops in the treatment of microstructural evolution, to achieve a physically consistent description of dynamics of complex dislocation microstructures. The selection and the implementation of internal degrees of freedom for large-scale simulations needs to be further discussed however, because the gained detail is always compensated by the computational cost. Another SDD model was developed by Martinez et al. 2019 (unpublished results). In that framework, the velocities are directly solved from the equation of dislocation motion associated with thermal agitation.

4 Collective/Massive DD simulations

Predicting the mechanical changes in irradiated materials is one long-term objective of applying the dislocation theory. One of the main challenges is bridging the huge time and length scale gaps existing from electronic structure calculations up to the mechanical response of bulk materials. Mesoscale simulations are therefore of pivotal significance in filling this gap between the atomistic and continuum mechanical modelling frameworks. Here we discuss some representative examples of massive DD simulations, which attempts to achieve this goal in irradiation scenarios.

4.1 Hardening and plasticity flow localization

Irradiation hardening of a metal is attributed to the interplay between material's structure and radiation defects, particularly dislocation loops as shown in Section 3. Along with the plastic deformation of many highly irradiated materials, it is often accompanied with another phenomenon known as the strain localization, whereby the movement of dislocations is concentrated in "defect-depleted" channels resulting in a highly spatially heterogeneous plastic flow (Victoria et al., 2000; Hashimoto et al., 2004; Byun and Farrell, 2004; Byun and Hashimoto, 2006; Zinkle and Singh, 2006). These channels have a typical width of several hundred of nanometers. The formation mechanism is generally interpreted by local removal (or absorption) of radiation defects by gliding dislocations.

DD simulations of bulk material, which enable a direct description on dislocationdefect interactions, therefore take advantages in modelling these phenomena and can provide insights in evaluating the hardening level and tracing the evolution of dislocation channels. DD simulations carried out by Nogaret et al. (2008) has shown the material strengthening and the clear band formation in Cu using absorption mechanisms between screw dislocations and faulted Frank loops informed from MD results. It is shown that loop absorption by screw dislocations is facilitated by the formation of extended dislocation pile-ups.

The work of Arsenlis et al. (2012) has then investigated the post-irradiation deformation in BCC Fe containing various concentrations of $1/2\langle 111 \rangle$ dislocation loops. These authors highlighted that yield stress increases obtained with various defect densities are in accordance with the disperse barrier hardening (DBH) model, where $\Delta \sigma_v = \alpha \mu b \sqrt{D\rho_D}$ with D the defect size, ρ_D the defect number density and α a defect strength coefficient. Limitations of this model have been furthermore discussed, stressing that the DBH model ignores the decoration effect on grown-in dislocations (source hardening) as part of the irradiation process. The disperse barrier effect is thus rationalized in terms of the minimum activation stress of dislocation sources through a homogeneous loop field. Moreover, the authors have shown that above a critical defect density, channels can be initiated by the formation of dislocation sources in defect-depleted regions. These new sources can grow up by absorbing and coalescing with more dislocation loops and move at much lower stresses compared to the region with homogeneous distributed loop field. Channels can then develop in an unstable manner, where the flow stress decrease associated with loop coalescence and absorption outweighs the flow stress increase due to network multiplication. Fig. 1.8a shows these dislocation channels with the orientation along the [211] direction, in an iron single crystal in presence of a defect dispersion with a density of $1.6 \times 10^{22} \text{ m}^{-3}$.

Post-irradiation tensile straining in Fe-grain in presence of $\langle 100 \rangle$ facet-loop dispersions with a density up to 5×10^{21} m⁻³ was investigated by Gururaj et al. (2015b). The temperature-independent consistence between the defect-induced hardening and the DBH model has been also validated. In addition, it was clearly seen that hardening levels significantly increased if accounting for the source hardening (dislocation decoration), which in turn triggered plastic flow localization earlier. Based on these results, authors reckoned

that the onset of plastic flow localization is more likely associated with the hardeningsoftening level, rather than the defect density per se. Further validations were reported in their following work (Gururaj et al., 2015a). Two types of DD simulations were performed in irradiated Cu, including simulations on the formation of single dislocation channels at a high resolution and the channel multiplication at the grain scale (see Fig. 1.8b), using prismatic dislocation loops and simplified fact-loops, respectively. From these simulations, it is concluded that the cross-slip is of particular importance in channel initiation and multiplication. Similar conclusions were obtained in DD simulations containing a combination of oxide-dispersed particles and irradiation defects. It was found that the particle/loop interplay can reduce the hardening level and delay the strain localization by generating high local internal stress around particles and enhancing the cross-slip activation (Gururaj and Robertson, 2011; Robertson and Gururaj, 2011).

Micro-mechanical measurements contribute to facilitating the assessment of dosedependent evolutions, since these tests requires handling much smaller amounts of radioactive materials. Extensive experiment and modelling results have shown that the specimen size has a pronounced influence on the mechanical response of tested materials (Csikor et al., 2007; Cui et al., 2016; Hosemann, 2018). For instance, it has found that the spatial correlation of dislocation microstructure and plastic deformation is significantly declined in the submicron regime, where dislocation interaction and cross slip are inhibited. DD simulations can naturally generate results at the length scale comparable to this sort of experimental testing. Using parametric DD methods coupled with a field description of nanoscale defects, Cui et al. (2018a) have quantitatively studied the size effect on the plastic flow localization in Fe micropillars. In Fig. 1.9, it is clearly seen that the dislocation channel width at the same plastic strain significantly decreases with the pillar size. At small scales, the flow localization transition from irradiation-defect clearing controlled to an intrinsic limited dislocation source dominated mechanism is clearly demonstrated. More details regarding the plastic flow in irradiated micropillars can be found in their following papers, in terms of material type (BCC Fe and FCC Cu), loading mode (strain and stress), and irradiation conditions (Cui et al., 2017, 2018b).

4.2 Effect on dislocation motion

In addition to materials hardening due to dislocation/defect interactions, dispersed radiation-generated defects strongly influence the effective mobility of dislocation populations as well. By implementing the appropriate dislocation mobility rules, DD simulations are beneficial for investigating the evolution of the dislocation motion in a quantitative manner. Hiratani and Zbib (2002) have shown the intermittent gliding motion of dislocations confronted with an array of SFTs using stochastic dislocation dynamics under various loading conditions. Their simulations revealed that the stress and temperature dependence of the average dislocation velocity transitions from an obstacle-controlled regime to a drag-controlled regime when the stress is above the critical resolved shear stress (CRSS). DD simulations of Li et al. (2019c) performed a systematic comparison between dislocation/loop interactions and equivalent dislocation/facet interactions for the sake of



a) Channels in Fe





FIGURE 1.8: DD simulation examples of channels. (a) Dislocation microstructure in an iron single crystal in presence of a defect dispersion with a density of 1.6×10^{22} m⁻³, showing defect-free dislocation channels (in blue). (From Arsenlis et al. 2012) (b) Plastic strain map of an irradiated copper grain populated with a density of 10^{22} m⁻³ facet-loops. The white dashed lines indicate the dislocation channel positions inside the underlying deformed grains. (From Gururaj et al. 2015a)

evaluating the effect of loop-induced stress fields on the dislocation motion. It is shown that screw dislocation mobility in presence of defect dispersions and cross slip can be ac-



FIGURE 1.9: Dislocation microstructures (red lines) in irradiated Fe micro-pillars with different diameters and irradiation defect (dark grey dots) number densities. Blue dotted regions denote dislocation channels. (Cui et al. PRL)

curately described using the facet-loop surrogate approach, which can in turn significantly improve the computational efficiency of massive DD simulations.

In BCC crystals, the impedient effect due to the defect dispersions could lead to embrittlement, resulting in the so-called ductile to brittle transition temperature shift (Δ DBTT, see also Section 5.1). The ductile to brittle (DBT) transition can be characterized using series of Charpy tests carried out at different temperatures (Brezis et al., 1999; Was, 2016). Therefore the general modelling of the DBTT focues on studying the macroscopic fracture of metals, using probability methods (e.g. Beremin model Beremin et al. 1983; Haušild et al. 2005a) or plasticity simulations (e.g. local approach and visco-plasticity Bouchet et al. 2005; Tanguy et al. 2006; Vincent et al. 2010).

As plastic deformation is mediated by dislocations, DD simulations is one of the few adapted methods, capable of addressing the damage-related plasticity mechanisms. The DD simulations of Li et al. (2019b) have shown a quantitative analysis on the motion of screw dislocation populations gliding through defect dispersions, accounting for thermally activated slip and cross-slip mechanisms. Ferritic grains with various defect dispersions were strained at a fixed temperature, and the defect-induced evolutions of the effective screw dislocation mobility were evaluated by means of statistical comparisons, using a proposed Defect-Induced Apparent Straining Temperature shift (Δ DIAT) concept. This concept can be interpreted as shown in Fig. 1.10. Dislocation/defect in-

teractions at a fixed straining temperature T_2 are equivalent to a definite temperature reduction $(T_2 - T_3)$, in terms of statistical, thermally activated screw dislocation velocities $(v_0 \rightarrow v_1)$. The radiation condition, straining temperature, grain size and grain orientation effects on the statistical evolutions of dislocation mobility have been furthermore studied. It is thereby found that the calculated Δ DIAT level closely matches the ductile to brittle transition temperature shift (Δ DBTT) associated with a given defect dispersion. The observed Δ DIAT/ Δ DBTT correlation is explained based on plastic strain spreading arguments indicating that the dose-dependent evolutions of the brittle to ductile transition are then possibly controlled by defect-induced changes of the effective dislocation mobility. A similar idea has proposed recently, based on an atomic-scale study, explaining the brittle-ductile transition depending on isolated dislocation/obstacle interactions (Swinburne and Dudarev, 2018).



FIGURE 1.10: Screw dislocation velocity as a function of effective stress for various straining temperatures. Markers 0 denote the un-irradiated case while markers 1 denote the irradiated case.

4.3 Other applications

Creep of metals proceeds with the relatively slow accumulation of plastic deformation under constant thermo-mechanical load conditions. Point defect production due to irradiation can strongly accelerate this process, resulting in so-called irradiation creep (Was, 2016; Nabarro and De Villiers, 2018). It is widely accepted that irradiation creep is closely connected with the climb of dislocations over obstacles and glide along slip planes, and thus amenable to study by DD simulations. In general DD frameworks, climb is implemented using an ad-hoc, conservative mobility coefficient, and this approach is not sufficient to capture all the involved physics in irradiation creep. In order to better analyze irradiation creep in the context of enhanced defect production, more elaborated diffusion-based models were developed and implemented in DD simulations. A heuristic method of dislocation climb controlled by bulk diffusion was developed by Mordehai et al. (2008, 2009). This model is based on the diffusion theory of vacancies, where the dislocation climb rate arising from the vacancy diffusion is obtained by solving Fick's equation locally. In this preliminary step towards the full modelling of creep, several elementary mechanisms, including activation of Bardenn-Herring sources, shrinkage and coarsening of prismatic loops have been evaluated under situations of pure climb without dislocation glide. Dislocation climb and glide were further implemented in a 3D nodal-based DD simulation by Bakó et al. (2011), using a similar dislocation climb model. Additional dislocation climb and glide model developments can be found in (Geslin et al., 2015; Gu et al., 2015). Using these models, extended creep simulations from dislocation dynamics were reported by Liu et al. (2014) and Keralavarma and Benzerga (2015). More recently, Gao et al. (2017) performed a 3D DD creep simulation, investigating the creep behaviour of Ni-based single crystal superalloys, which considered dislocation glide, climb and vacancy diffusion explicitly. It is found that plastic deformation is mainly controlled by dislocation glide in γ -matrix channels, while the effect of the dislocation climb, which is a temperature and stress dependent process, leads to the stress relaxation by rearranging the dislocation configuration as shown in Fig. 1.11.

Another application of DD simulations is in aspects of H embitterment (HE) problem of metals, which is in a position to accurately probe dislocation microstructure evolutions in H environment. As H strongly affects dislocation emission, dislocation nucleation and dislocation mobility, DD simulations of this specific problem requires incorporating these H effects in an efficient manner (Tarleton, 2019). Inspired from atomistic calculations, Gu et al. (2018) have introduced Hydrogen into DD framework, wherein H atoms were treated as point-like misfitting inclusions in an infinite elastic volume. The stress induced by H atom is evaluated in equilibrium conditions with respect to the dislocation stress field. Hdislocation interaction is accounted for by the first order elastic interaction energy term. This model was then applied to study the role of H on a gliding dislocation loop and the arrangement of parallel dislocations. A shielding effect was observed in materials having a large hydrogen diffusivity, e.g. in BCC iron, which resulted in the homogenization of the loop shrinkage and the decrease in the spacing of parallel edge dislocations, consistent with hydrogen elastic shielding theory. This model was furthermore extended to a finite boundary value problem by Yu et al. (2019) using the superposition principle, whereby the plastic deformation was studied in a microcantilever beam through DD simulations. It is found that hydrogen can promote dislocation activity which lowered the flow stress and generated more pronounced slip steps on the free surfaces, consistent with the hydrogen enhanced localized plasticity (HELP) mechanism.



FIGURE 1.11: Dislocation configurations in γ -matrix channels in two simulations with and without dislocation climb. The colors of the dislocation segments indicate the different FCC slip systems. (From Gao et al. 2017)

5 Overview and organization of the thesis

5.1 **RPV steel : chemical composition and mechanical response**

The reactor pressure vessel (RPV) is considered as the primary structural component in nuclear power reactors, which serves as an essential barrier against the radioactivity outlet. In this section we present some properties of RPV steel.

The French RPV is made with industrial low alloyed steel 16MND5 of bainitic structure. And the chemical composition of French RPV steel as specified by the French code of design and construction (RCC-M) is indicated below (Vieillard-Baron and Meyzaud, 1998). Each alloying element has a specific effect on the microstructure and the final properties of the pressure vessel.

TABLE 1.1: Chemical composition of RPV in French nuclear reactors in weight precent as specified in the French code of design and construction (RCC-M Vieillard-Baron and Meyzaud 1998).

С	Mn	Ni	Мо	Cr	Р	S	Si	Al, Co
0.16	1.15-1.55	0.5-0.8	0.45-0.55	0.25	0.008	0.005	0.1-0.3	<0.1

The microstructure of the RPV steel is comprised of lath bundles, or in the form of individual plates. Observations of the banitic microstructure of 16MND5 RPV steel

is done by optical microscope and scanning electron microscope (SEM), as shown in Fig. 1.12.



FIGURE 1.12: Bainitic microstructure of 16MND5 RPV steel. Observed with optical microscope (left) amd SEM (right). The dark constituent is a bundle of bainitic ferrite laths, while the lighter phase is made of carbides. (From Hausĭld 2002)

The RPV steel has a body-centered cubic (BCC) crystallographic structure, the stressstrain relation is therefore affected by temperature as shown in Fig. 1.13. It is seen that the yield stress and the fracture stress decrease when temperature increases. The latter is associated with the ductile to brittle transition (DBT).



FIGURE 1.13: Stress-strain curve for 16MND5 steel at different temperatures under a strain rate of 5×10^{-4} s⁻¹. (From Libert 2007)

Subjected to neutron irradiation, RPV steel undergoes several mechanical properties degradations including radiation induced hardening and embrittlement as shown in

Fig. 1.14. Fig. 1.14a illustrates the increase in the yield stress of the RPV steel due to the neutron irradiation. Fig. 1.14 shows the DBT temperature shift.



FIGURE 1.14: Radiation effects on RPV steel. (a) Stress-strain curve. (From Haušild et al. 2005b) (b) Ductile to brittle transition. (From Bouchet et al. 2005)

5.2 organization of the thesis

As the post-irradiated plastic deformation is mediated by dislocations, dislocation dynamics simulation method is here applied in an attempt to investigate the microstructure evolution and mechanical property change in RPV steels. New insights on how prismatic loops affect post-irradiation scenarios will be presented first, with a particular emphasis laid on studying their interactions with the surrounding dislocation microstructures. Specific effort is then paid on evaluating their impact on the overall microstructural evolution and plastic deformation of iron-based metals. The dissertation is organized as follows:

Chapter 2 shows how to simulate diffusion of prismatic loops with $a/2 \langle 111 \rangle$ -type Burgers vectors in BCC iron using the discrete dislocation dynamics approach, accounting for the elastic forces acting between the loops and stochastic forces associated with the ambient thermal fluctuations. An expression for thermal stochastic forces acting on a dislocation line is derived. The fluctuation-dissipation theorem, which relates the amplitude of stochastic thermal forces to the magnitude of the dissipative drag effect experienced by a dislocation moving through a crystal, is further discussed with the purpose of validating the simulation results. Finally, the elementary loop-loop reactions are simulated, together with investigations of the loop tilting effect on the loop diffusing dynamics.

Chapter 3 elucidates the cross-slip effect on dislocation/defect interactions in BCC iron, assessed by means of specific three-dimensional nodal DD simulation setups, in consistence with available experimental evidence of cross-slip activity in post-irradiation straining conditions. The interaction mechanism and the corresponding critical stress are analyzed in cases of interactions between screw-type dislocation sources and two types

of prismatic loops. The influence of the loop-induced stress field on such interactions has been furthermore highlighted by comparisons between simulation setups where the loops have been replaced by hard impenetrable facets. The final purpose of this work is to distinguish if the loop-facet is an efficient surrogate to the actual dislocation loop.

Chapter 4 treats the post-irradiation plastic strain spreading of ferritic grains in presence of defect dispersions, using segment-based DD simulations. Each simulated irradiation condition is characterized by the aforementioned Defect-Induced Apparent Temperature Shift (Δ DIAT) concept, reflecting the statistical evolutions of screw dislocation mobility. And the obtained Δ DIAT levels are further compared to the measured ductile to brittle transition temperature shift (Δ DBTT). The ultimate objective of this work is to develop an embrittlement model that can be utilized in combination with conventional nuclear surveillance techniques, in an attemp to facilitate the prediction of dose-dependent Δ DBTT evolutions.

Chapter 2

Diffusion and interaction of prismatic dislocation loops

This chapter is reproduced from:

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Body-centred cubic metals and alloys irradiated by energetic particles form highly mobile prismatic dislocation loops with $a/2\langle 111 \rangle$ -type Burgers vectors, as evidenced by in-situ transmission electron microscopy (TEM) observations. The one-dimensional migration and correlated motion of these dislocation loops, often observed experimentally, are an elementary process leading to the formation of rafts of defects. The subject of this chapter is the simulation of stochastic glide motion of prismatic $a/2\langle 111 \rangle$ dislocation loops, with a particular emphasis on the analysis of elementary reactions between the loops, treated as dislocation line objects, and modelled using discrete dislocation dynamics. The influences of the interplay between stochastic thermal forces and internal degrees of freedom of loops, in particular the reorientation of the loop habit planes, on the observed loop dynamics have been furthermore examined, in terms of the interaction energy of loop-pair cases.

1 Introduction

Metals exposed to irradiation develop a highly complex microstructure, involving a mixture of mobile and immobile defects of both interstitial and vacancy type. The defect and dislocation network develops under the effect of internal and external stresses and temperature, and generates its own fluctuating stress field, leading to a variety of changes
in mechanical properties, such as hardening and the loss of ductility, and having a detrimental effect on the longevity of structural reactor components in a radiation environment.

Predicting the dynamics of evolution of microstructure is a major challenge to computer modelling because of the broad spectrum of activation energies characterizing defect and dislocation networks. Defect cluster migration barriers vary from meVs to eVs. The binding energy of elastically confined defect structures spans a similar range of energy scales (Dudarev et al., 2010), and the magnitude of elastic interaction depends on the size of defects and their spatial distribution. Simulating the temperature dependent dynamics of microstructure requires the treatment of intrinsic thermally activated Brownian motion of defects and dislocations, as well as correlated motion of defects and dislocations mediated by elastic interactions.

Highly glissile prismatic dislocation loops are produced by irradiation (Barnes, 1963; Arakawa et al., 2007) together with sessile cavities, as evidenced by *in-situ* transmission electron microscopy (TEM) observations (Zinkle and Singh, 2006; Jenkins et al., 2009). The correlated motion of dislocation loops, often observed experimentally, is an elementary process leading to the formation of rafts of defects and their eventual coalescence (Yao et al., 2008; Hernández-Mayoral et al., 2008; Arakawa et al., 2011; Dudarev et al., 2014). In other words, the spatial ordering of dislocation loops stems from their elastic interaction, whereas the loop motion itself is a thermally activated process, fundamentally the same as stochastic Brownian motion of individual defects (Wirth et al., 1997; Osetsky et al., 1999, 2003; Dudarev, 2008; Dudarev et al., 2014; Swinburne et al., 2016). The subject of this paper is the simulation of stochastic glide motion of prismatic $a/2 \langle 111 \rangle$ dislocation loops in body-centered cubic (BCC) iron, with a particular emphasis on the analysis of elementary reactions between the loops, treated as dislocation line objects, and modelled using discrete dislocation dynamics.

Molecular dynamics and lattice type simulations performed over the past two decades investigated the stochastic diffusion of prismatic loops over a range of sizes and temperatures (Wirth et al., 1997; Osetsky et al., 1999; Wirth et al., 2000; Marian et al., 2002; Osetsky et al., 2003; Anento et al., 2010; Derlet et al., 2011), elementary loop and dislocation reactions (Dudarev et al., 2010, 2014), as well as energies of binding of loops to other defects (Domain and Becquart, 2018). However, a direct atomistic simulation of an ensemble of interacting dislocation loops still remains a challenge because of the constraint imposed by the simulation cell size accessible to a molecular dynamics simulation, and the relatively short timescale of such a simulation. While the more recent atomistic approaches involving the use of kinetic Monte Carlo (Xu et al., 2012; Mason et al., 2014; Béland et al., 2015a,b) have reached the experimentally relevant time scale when exploring the relaxation of radiation cascade damage in thin films, the identification of pathways of migration and reaction between interacting dislocation loops containing more than a few dozen interstitials remains a largely unexplored problem.

Discrete dislocation dynamics (DDD) provides a compelling alternative approach to modelling complex dislocation microstructures, offering highly efficient computation of long-range elastic interactions. Furthermore, dislocation dynamics enables the treatment of dislocation reactions, simultaneously simulating internal and collective dislocation loop dynamics and enabling the investigation of complex networks and junctions within the same methodological framework. We note that it remains a considerable challenge to bring dislocation core properties on par with atomistic simulations, see the recent extensive developments addressing this issue (Fitzgerald, 2016; Boleininger et al., 2018; Geslin and Rodney, 2018; Zhang and Ngan, 2018; Po et al., 2018).

The objective of this work is to include thermal stochastic forces in DDD through the Langevin stochastic formalism, to enable modelling the Brownian diffusion of dislocations. The stochastic dislocation dynamics (Hiratani and Zbib, 2002, 2003) approach is formulated and applied to the treatment of diffusion of loops and elementary reactions between interacting loops as an essential step towards modelling thermal evolution of complex dislocation ensembles.

Langevin dynamics has been applied earlier to the treatment of collective dynamics of dislocation loops on a coarse-grained level, where the loops were treated as point-like objects interacting through long-range elastic fields described in the elastic dipole tensor approximation (Dudarev et al., 2010, 2014; Dudarev and Sutton, 2017; Dudarev and Ma, 2018). Extending the treatment to the case where loop dynamics involves also the relaxation of their internal degrees of freedom, such as tilting of the loop habit plane, we find that this strongly increases the lifetime of configurations where pairs of loops are bound together by their attractive elastic fields. Furthermore, the barriers to entering such bound states are strongly reduced, explaining why dislocation loop rafts are able to form so easily in many materials, as confirmed by *in-situ* TEM observations (Dudarev et al., 2010, 2014; Yi et al., 2015).

The paper is organized as follows. In Section 2 we derive an expression for thermal stochastic forces acting on a dislocation line. In Section 3 the diffusion coefficient of a single prismatic loop is evaluated and examined as a function of temperature, and the DDD analysis is benchmarked against molecular dynamics simulations. We also discuss the fluctuation-dissipation theorem, relating the amplitude of stochastic thermal forces to the magnitude of dissipative drag experienced by a dislocation moving through a crystal. Next, the concept of the loop-loop interaction potential energy surface is introduced, and the elementary loop-loop reactions are simulated, with particular attention devoted to the investigation of internal degrees of freedom of the loops. Finally, in Section 4 we evaluate the lifetime of an elastically confined loop-loop configuration, which is a functional of the loop-loop interaction potential energy surface.

2 Simulation method

2.1 Stochastic force in dislocation dynamics

All simulations described in this paper were performed using the 3D nodal dislocation dynamics code NUMODIS (Drouet et al., 2014). In NUMODIS, continuous dislocation lines are discretized into a series of nodes linked by straight dislocation segments. The internal elastic stress is then computed according to the non-singular isotropic elasticity theory (Cai et al., 2006). The Langevin equation of motion for every point on a dislocation segment is based on the dynamic equation of motion, taken here in the overdamped limit (Bulatov and Cai, 2006):

$$\underline{B} \cdot \boldsymbol{v} = \boldsymbol{f}^{tot} + \boldsymbol{f}^s, \tag{2.1}$$

where v is the velocity of the dislocation line, $\underline{\underline{B}}$ is the viscous drag tensor per dislocation line unit length depending on the slip system and temperature, and f^s is the stochastic force per unit length. The stochastic force acts to introduce transient thermal fluctuations into the dislocation network in order to simulate the coupling between the dislocations with the heat bath represented by the surrounding crystal lattice.

The total configurational force per unit length f^{tot} exerted on a dislocation segment equals

$$\boldsymbol{f}^{tot} = \boldsymbol{f}^{el} - \boldsymbol{\nabla} \boldsymbol{E}^{core}.$$
(2.2)

In the absence of external body and image forces, the elastic driving force reduces to the well-known Peach-Koehler (PK) force. The core energy E^{core} is a phenomenological correction introduced to describe the effect of non-linear interaction in the dislocation core region, which is not accounted for by linear elasticity theory. The core energy is also required to yield a net positive line-tension for small-scale line fluctuations (Szajewski et al., 2015; Geslin and Rodney, 2018), which are expected to arise from the action of stochastic force. The core energy per unit length of a dislocation line is here given in the line-tension approximation (Dupuy and Fivel, 2002)

$$E^{core} = \frac{\xi \mu b^2}{4\pi (1-\nu)} \left(1 - \nu \cos^2 \psi(l)\right), \qquad (2.3)$$

where ξ is the core strength parameter, ψ is the angle between the dislocation tangent and the Burgers vector, and *l* is the coordinate of a point on a dislocation line.

Consider the intrinsic mobility of an individual prismatic loop with perimeter L in an infinite medium in the absence of external forces. Without loss of generality, assume that the Burgers vector of the loop is collinear with the z direction of the Cartesian system of coordinates. In the absence of climb forces, the motion for a dislocation line is one-dimensional

$$B\frac{\partial z(l,t)}{\partial t} = f_z^{tot}(l,t) + f^s(l,t), \qquad (2.4)$$

where B is the viscous drag coefficient for the given slip system and the stochastic force f^s is assumed to be uncorrelated in time and space:

$$\langle f^{s}(l,t)\rangle = 0, \langle f^{s}(l,t)f^{s}(l',t')\rangle = \sigma_{s}^{2}\delta(l-l')\delta(t-t'),$$

$$(2.5)$$

where σ_s sets the scale of the stochastic force, and $\delta(x)$ is the Dirac delta-function

$$\delta(x) = 0, \quad \forall x \neq 0,$$

$$\int_{-\infty}^{\infty} dx \, \delta(x) = 1.$$
 (2.6)

To find the amplitude of stochastic force, the effective diffusion coefficient for the center-of-position (COP) of the prismatic loop is matched to a 1D Einstein diffusion law (Derlet et al., 2011). The projection of the COP on the Burgers vector direction is given by $z_{\text{COP}} = L^{-1} \int_0^L dl \ z(l,t)$. After a rearrangement, Eq. (2.4) becomes

$$\frac{\partial z_{\text{COP}}}{\partial t} = \frac{1}{BL} \int_0^L \mathrm{d}l \ f^s(l,t). \tag{2.7}$$

The effect of internal elastic force on the COP vanishes due to the boundary condition z(l+L,t) = z(l,t). Assuming that the initial position of the loop center is $z_{COP}(0) = 0$, the solution to Eq. (2.7) at time τ is

$$z_{\rm COP}(\tau) = \frac{1}{BL} \int_0^L dl \int_0^\tau dt \ f^s(l,t).$$
(2.8)

Since the stochastic force $f^{s}(l,t)$ is defined in terms of its correlation function, the mean square displacement of the COP can be expressed as

$$\left\langle z_{\text{COP}}^{2}(\tau) \right\rangle = \left(\frac{1}{BL}\right)^{2} \int_{0}^{L} dl \int_{0}^{L} dl' \times \int_{0}^{\tau} dt \int_{0}^{\tau} dt' \left\langle f^{s}(l,t) f^{s}(l',t') \right\rangle.$$
(2.9)

Substituting Eq. (2.5) into Eq. (2.9) yields

$$\langle z_{\text{COP}}^2(\tau) \rangle = \left(\frac{\sigma_s}{BL}\right)^2 \int_0^L dl \int_0^L dl' \times \int_0^\tau dt \int_0^\tau dt' \delta(l-l') \delta(t-t').$$
 (2.10)

Evaluating the above integral, we arrive at

$$\langle z_{\rm COP}^2(\tau) \rangle = \left(\frac{\sigma_s}{BL}\right)^2 L \tau \equiv 2D_{\rm COP} \tau.$$
 (2.11)

This equation is a mere corollary of the 1D Einstein diffusion law, where D_{COP} is the corresponding diffusion coefficient of the centre-of-position (Pécseli, 2000). Substituting the fluctuation-dissipation relation

$$D_{\rm COP} = \frac{k_{\rm B}T}{BL} \tag{2.12}$$

into Eq. (2.11), which holds under the assumption that the dislocation loop is in thermodynamic equilibrium with the thermostat, we find the amplitude of the stochastic force

$$\sigma_s = \sqrt{2k_{\rm B}TB},\tag{2.13}$$

where $k_{\rm B}$ is the Boltzmann constant and T is absolute temperature.

As NUMODIS is a nodal dislocation dynamics code, the total force per unit length is converted into an effective nodal force by integrating over the neighboring segments (Bulatov and Cai, 2006). The same rule is applied to convert the stochastic force per unit length into a stochastic force acting on a node. However, care must be taken when rescaling the force, as the randomly applied force must remain consistent with the choice of the segment length and the integration time step. For a straight segment of length Δl indexed by *n*, the scaled stochastic force per unit length is found using the stochastic average:

$$f_n^s(t) = \frac{1}{\Delta l} \int_{l_n - \Delta l/2}^{l_n + \Delta l/2} \mathrm{d}l \ f^s(l, t).$$
(2.14)

Using Eq. (2.5), for the δ -correlated force generated by thermal fluctuations, the nodal correlation function acquires the form

$$\left\langle f_n^s(t) f_{n'}^s(t') \right\rangle = \frac{\sigma_s^2}{(\Delta l)^2} \int_{l_n - \Delta l/2}^{l_n + \Delta l/2} \mathrm{d}l \int_{l_{n'} - \Delta l/2}^{l_{n'} + \Delta l/2} \mathrm{d}l' \\ \times \delta(l - l') \delta(t - t')$$

$$= \frac{\sigma_s^2}{\Delta l} \delta_{n,n'} \delta(t - t').$$

$$(2.15)$$

Similarly, assuming an integration time step of Δt , the scaled stochastic force per unit length can be finally expressed as

$$f_n^s = \sqrt{\frac{2k_{\rm B}TB}{\Delta l\Delta t}} N(0,1), \qquad (2.16)$$

where N(0,1) is a random number sampled from the standard normal distribution, and the direction of the force is collinear with the Burgers vector of the dislocation loop.

2.2 Simulation setup, parameters, and statistics

All the dislocation dynamics (DD) simulations were performed assuming an infinite medium. The coordinate system is chosen as orthogonal with axes parallel to $x = [\overline{112}]$, $y = [1\overline{10}]$, and z = [111] directions. Initially, a hexagonal prismatic $\langle 111 \rangle$ dislocation loop is positioned at the origin. The loop radius is chosen as $\rho = 4.5$ nm, corresponding to the loop perimeter of L = 27 nm. The hexagonal loop shape was chosen out of convenience as this has an almost negligible effect on its dynamics. A round loop of equivalent size would have the radius of 4.09 nm, representing an inclusion of equal amount of matter.

The three parameters included in the stochastic force (2.16) require further clarification.

The viscous drag coefficient *B* characterizes the drag force acting on a dislocation line. In bcc metals it is generally assumed that $B(T) = B_0 + B_1 T$, where B_0 and B_1 are independent of temperature (Swinburne et al., 2014; Swinburne and Dudarev, 2015; Po et al., 2016). MD simulations of glissile prismatic loops and self-interstitial clusters in



FIGURE 2.1: Viscous drag coefficient *B* for a prismatic dislocation loop in BCC iron extracted from molecular dynamics simulations (Derlet et al., 2011) (dots). The viscosity is well described by a non-Arrhenius relation (line), see Derlet et al. (2011) for the choice of parameters in the functional expression ($D_0 = 392.69 \times 10^{-10} \text{ m}^2/\text{s}$, E = 0.0386 eV). The dashed line corresponds to the constant value of $B = 0.08 \text{ MPa} \cdot \text{ns}$ used here, which is valid for temperatures above 200 K.

bcc metals show that $B(T) = B_0$ and is independent of T over a wide temperature range. Given that the simulations performed in this study address prismatic dislocation loops of very small size, it is appropriate to treat B as a temperature-independent constant. The numerical value of B used in this work has been evaluated from the atomistic study by Derlet et al. (2011) using the fluctuation-dissipation relation (2.12). The resulting value of the drag coefficient B = 0.08 MPa \cdot ns describes the effective mobility of edge dislocations at temperatures above T = 200 K, but underestimates the magnitude of drag at lower temperatures, as shown in Fig. 2.1. At low temperatures, the Peierls barrier (Ohsawa and Kuramoto, 2007; Swinburne, 2013) and quantum effects (Proville et al., 2012; Swinburne et al., 2017) play an important part, affecting dislocation mobility, but are not considered in this study. The chosen value of B = 0.08 MPa \cdot ns agrees well with previous parameterizations derived from the analysis of dislocation-defect interactions in BCC iron (Shi et al., 2015; Li et al., 2018).

Since the simulations were performed by splitting dislocation loops into straight segments, and involved solving the equations of motion by means of a finite difference time integration algorithm, it would be appropriate to assess the effect of discretization length Δl and time step Δt on the computed diffusion coefficient. Thermal diffusion of a single prismatic loop at 300 K was simulated using three discretization lengths, $\Delta l = 5, 10$, and 15 Å, and three time steps, $\Delta t = 0.2, 0.5$ and 1.0 fs. Simulations were run over the interval of 6 ns, with the loop configuration data recorded every 0.6 ps. The loop diffusion coefficients were computed using the drift diffusion correction method (Derlet et al., 2011), in which the diffusion trajectory was split into N uncorrelated sub-trajectories $z_{COP}^{(i)}(t)$:

$$D_{COP} = \frac{3}{2t_0} \left\langle \left(z_{COP}^{(i)}(t_0) - \frac{2}{t_0} \int_0^{t_0} d\tau z_{COP}^{(i)}(\tau) \right)^2 \right\rangle,$$
(2.17)

where t_0 is the sub-trajectory time. The expectation value is taken over all sub-trajectories, hence the standard error of the mean of the diffusion constant is given as

$$D_{COP} = \langle D_{COP} \rangle \pm \langle D_{COP} \rangle / \sqrt{N}.$$
(2.18)

The velocity auto-correlation function $\langle v_{COP}(t)v_{COP}(t+\tau)\rangle$ yields the correlation time of $\tau \approx 2$ ps, in broad agreement with atomistic estimates (Dudarev, 2008; Geslin and Rodney, 2018). The velocity correlation time is longer than the stochastic force correlation time (Swinburne et al., 2014) derived from atomistic simulations, and represents the low limit for the time length of a sub-trajectory, which here was chosen as 6 ps. The diffusion coefficient is then found by ensemble averaging over the sub-trajectories, with the uncertainty characterized by the standard error of the mean.

Fig. 2.2 shows a selection of simulated COP trajectories, which are similar in terms of their statistical properties. The values of diffusion coefficient derived from these trajectories remain within their respective error bounds, independent of the selected values of Δl and Δt , in agreement with the theoretical analysis by Derlet et al. (2011).

Following Scattergood and Bacon (1975), the elastic moduli μ and v are chosen by matching the isotropic and anisotropic elasticity energies of infinite $a/2 \langle 111 \rangle \{110\}$ edge and screw dislocations. Earlier comprehensive studies (Han et al., 2003; Yin et al., 2010; Fitzgerald and Aubry, 2010) confirm that this method leads to highly accurate predictions of dislocation loop shapes and stress fields. In this work, the anisotropic moduli used as input were chosen following Ackland et al. (2004) as $C_{11} = 225$ GPa, $C_{12} = 124$ GPa, and $C_{44} = 101$ GPa, leading to the corresponding isotropic moduli of $\mu = 63$ GPa and v = 0.43. The dislocation core radius R_c (Cai et al., 2006), here used as the spreading radius for nonsingular elasticity theory, and the core strength parameter ξ were parametrized in earlier work (Shi, 2014; Shi et al., 2015) by comparison with atomistic simulations.

The choice of isotropic elasticity theory represents an approximation for BCC iron, which is an elastically anisotropic material. The numerical results presented in this work are therefore to be interpreted qualitatively. However, this is a foregone conclusion if we acknowledge that common models of core energy do not tend to capture the complex configurational energy landscape found in atomistic simulations. The formalism for stochastic forces itself is directly transferable to DDD in anisotropic materials.

All the further simulations presented in Section 3 were carried out using the simulation parameters given in Tab. 2.1, unless specified otherwise.



FIGURE 2.2: Random walk trajectories of a prismatic loop with radius $\rho = 4.5$ nm undergoing Brownian motion at 300 K simulated using the same viscous drag coefficient, and several different discretization lengths Δl and time steps Δt . The diffusion behaviour of the loop is independent of the choice of discretization parameters.

3 Results

3.1 Stochastic dynamics of an individual dislocation loop

Using stochastic dislocation dynamics, we performed a series of simulations, investigating the dynamics of a single prismatic loop at temperatures ranging from 100 K to 800 K, with temperature increments of 100 K. No external stress was applied.

Consider first the internal degrees of freedom of the prismatic loop. It is readily seen from simulations that the initially purely prismatic [111] loop with its Burgers vector nor-

parameter	symbol	value
Burgers vector	b	2.47 Å
Shear modulus	μ	63 GPa
Poisson's ratio	ν	0.43
Drag coefficient	В	0.08 MPa · ns
Dislocation core radius	R_c	1.4 Å
Core strength parameter	ξ	0.257
Time step	Δt	0.5 fs
Discretization length	Δl	10 Å

TABLE 2.1: Simulation parameters for pure iron. (Shi, 2014; Shi et al., 2015)

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mal to its habit plane, within a few picosecond adopts a tilted configuration, see Fig. 2.3a. If the shape of the loop is defined by its dislocation countour C, the vector area of the loop is given by (Landau and Lifshitz, 1970; Dudarev and Ma, 2018)

$$\boldsymbol{A} = \frac{1}{2} \oint_{C} \boldsymbol{r} \times \mathrm{d}\boldsymbol{l}. \tag{2.19}$$

and the effective loop normal unit vector is

$$\hat{\boldsymbol{n}} = \frac{1}{2|\boldsymbol{A}|} \oint_{C} \boldsymbol{r} \times \mathrm{d}\boldsymbol{l}.$$
(2.20)

The angle between the Burgers vector and the effective loop normal shall be referred to as the tilt angle θ , with the azimuthal angle ϕ defined in full analogy with the spherical system of coordinates, see Fig. 2.3b for illustration. Following this definition and depending on the nature of the loop (vacancy or interstitial), the loop is pure prismatic if $\hat{n} \cdot \hat{b} = \pm 1$ corresponding to $\theta = 0$ or 180° . We note that the elastic relaxation volume of a loop is given by the scalar product of the Burgers vector and the loop vector area $\Omega_{rel} = b \cdot A$ (Dudarev and Ma, 2018).

The elastic potential energy of a prismatic loop is minimised for configurations tilted away from the perfect prismatic loop orientation, with the resulting tilt angle θ determined by the competition between the elastic self-energy associated with interaction between dislocation segments and the core energy proportional to the length of the perimeter of the loop, see Fig. 2.3c. The potential energy is invariant with respect to rotations around the Burgers vector, allowing the loop to rotate freely with respect to ϕ in a DD simulation.

The mean value of the tilting angle $\langle \theta \rangle$ decreases at higher temperatures, reflecting the anharmonicity of the potential self-energy of the loop. Indeed, it takes comparatively less energy for the loop normal to tilt towards the Burgers vector than away from it, hence on average smaller values of θ are favoured at higher temperature.

In addition to the tilting degrees of freedom, the loop shape also develops transient fluctuations on a smaller scale. However, any part of the loop is constrained to remain on the glide cylinder, as the relaxation volume of the loop $\Omega_{rel} = \mathbf{A} \cdot \mathbf{b}$ is conserved throughout the simulation.

Consider next the diffusion behaviour of the entire loop. The prismatic loop trajectories exhibit a characteristic pattern of Brownian motion, with higher temperature inducing a more pronounced loop displacement per unit time. The single loop COP trajectories for 200 K and 600 K, and the diffusion coefficients calculated with the drift diffusion correction (Derlet et al., 2011), are given in Fig. 2.4. Globally, the temperature dependence of the diffusion coefficient is found to be consistent with the fluctuation-dissipation theorem, regardless of the loop radius ρ .

Moreover, for $\rho = 4.5 \text{ nm}$ and T < 400 K the diffusion coefficients derived from simulations are consistently lower than expected from the linear interpolation from higher temperature (dashed line) because the tilting of the loop results in the elongation of its perimeter, see Fig. 2.3b. According to the fluctuation-dissipation theorem, $D_{\text{COP}} \propto 1/L$,



FIGURE 2.3: (a) Snapshots from a stochastic dislocation dynamics simulation of a hexagonal initially pure prismatic loop of 4.5 nm radius at 100 K show that the loop habit plane becomes tilted within a few picoseconds. (b) The tilt angle θ is defined as the angle between the normal vector (red arrow) and the Burgers vector (black arrow). (c) The prismatic loop adopts a tilted configuration on the glide cylinder to minimize its potential energy.

and therefore the reorientation of the habit plane gives rise to a lower value of the diffusion coefficient. This effect is found to become less pronounced at higher temperature as the mean tilt angle $\langle \theta \rangle$ decreases with temperature.

The stochastic DD simulations performed in this work describe thermally induced Brownian motion of prismatic loops, which for T > 200 K is consistent with molecular dynamics. The simulations further reveal that the prismatic loop habit plane becomes tilted with respect to the Burgers vector, while remaining highly mobile with respect to rotations around the Burgers vector.

The tilting behaviour of prismatic loops, also observed in atomistic simulations, is possibly dominated by singular orientation effects in the core energy (Kang et al., 2012). Considering that the core energy scales linearly with the loop radius $\propto \rho$, whereas the elastic self-energy varies super-linearly as $\propto \rho \log \rho$ (Anderson et al., 2017), one would expect the core energy to become less significant for larger loops. However, the singular nature of the core energy in combination with atomic discreteness would break the cylindrical symmetry of the system, subsequently introducing energy barriers in relation to its rotation around the Burgers vector.

3.2 Diffusion of interacting dislocation loops

The question about thermal evolution of interacting dislocation loops has recently attracted attention in the context of dipole tensor formalism as an efficient approximation for the long range elastic interaction between the loops (Dudarev and Sutton, 2017; Clouet et al., 2018). Here, we show that the internal degrees of freedom of loops, not explicitly treated by the dipole tensor formalism, have a profound effect on the stochastic dynamics of loops, particularly where the loops form bound configurations confined by attractive elastic interactions.

Consider a pair of prismatic loops with unit Burgers vectors $\hat{b}_1 = \hat{b}_2 = \hat{z}$. The loop centers are separated by distance *s* in the glide direction and by Δx in the direction perpendicular to the Burgers vector direction, see Fig. 2.5a. In the absence of climb force, either loop can move or distort only in the glide direction.

While the stochastic simulations involve an explicit treatment of internal degrees of freedom of the loops, it is also instructive to consider the static properties of a simplified system of two loops. Following the discussion in Section 3.1, the internal degrees of freedom of the simplified system are reduced to the tilting modes only, thus keeping the loops otherwise flat and of ellipsoidal shape.

For a single loop the potential energy is invariant with respect to rotations around its Burgers vector. For a pair of loops the invariance is lifted by their elastic interaction : for a loop-pair separation constrained at *s*, the system has multiple tilting configurations corresponding to local energy minima, giving rise to a complex potential energy surface (PES) with several branches and crossing points. In full analogy to the Born-Oppenheimer approximation of quantum physics (Ullrich, 2012), the internal degrees of freedom of loops evolve significantly faster (on the timescale of \sim ps) than the loop-pair separation (varying on the \sim ns timescale), and thus the notion of PES describes the system of in-



FIGURE 2.4: Top : Random walk trajectories of a hexagonal prismatic loop of radius $\rho = 4.5$ nm simulated for 200 K and 600 K. Bottom : Plots of diffusion coefficients as a function of temperature for different loop sizes ρ . Dashed lines are analytical predictions derived from the fluctuation-dissipation theorem $D_{\text{COP}} = k_{\text{B}}T/(BL)$.



FIGURE 2.5: (a) Two prismatic loops defined using the coordinate system introduced in Sec. 3.2, with identical Burgers vectors b parallel to z-direction. Loop configuration (line) is free to deviate from the pure prismatic form (dashed) on the glide cylinder, as indicated by the loop normal vectors \hat{n} . (b) A selection of representative metastable configurations of interacting loops extracted from dislocation dynamics simulations, also showing the loop normal and Burgers vectors. Configurations are ordered from top to bottom in the order of increasing stability, and hence in the order of descending total potential energy. Configuration 3 is the most stable configuration.

teracting loops in the adiabatic approximation. Each PES branch represents a meta-stable tilting state for a given reaction coordinate *s*. Transitions between PES branches occur by the rotation of loop habit planes, which are therefore separated by energy barriers.

The energy of interaction between pairs of prismatic loops is computed in the order of ascending accuracy: in the dipole tensor approximation for a pair of pure prismatic loops, as exact elastic interaction between a pair of pure prismatic loops, and as exact elastic interaction between prismatic loops with relaxed internal degrees of freedom. Note that in the dipole tensor approximation the expression for the loop-loop interaction reduces to the Foreman-Eshelby expression (Foreman and Eshelby, 1962; Barnes, 1963; Dudarev et al., 2010). The treatment of internal relaxation is explained in detail in Appendix A. The energy of interaction between the loops is defined as the energy difference between the total energy of two loops minus the energy of isolated loops with the same orientation of the Burgers vector.

$$W^{int}(s) = W^{tot}(s) - \lim_{s \to \infty} W^{tot}(s).$$
(2.21)

Energies of elastic interaction are compared in Fig. 2.6 for the various loop separations Δx using an example of two round loops with radii $\rho = 4.09$ nm. Note that the choice of radii is consistent with loops being hexagonal and having the same area, as discussed in Section 2.2.

The exact interaction energy trend for pure prismatic pairs of loops broadly follows the PES trend, but does not reflect the full complexity of interaction between internally relaxed loops. The dipole approximation is consistent with the exact treatment, but only for loop separations several times larger than the sum of loop radii. The dipole tensor formalism becomes inaccurate for smaller separations, resulting in a qualitatively incorrect predicted interaction behavior, see the top two panels in Fig. 2.6.

A major effect of internal relaxation is found when we follow how the loops approach an elastically confined bound state from infinite separation. This reaction is fundamental to the formation of dislocation loop rafts. From Fig. 2.6 it is evident that loop interaction energy at large separations is positive. Therefore an energy barrier first has to be overcome before the loops can enter a bound state. This barrier is here given by the maximum value of the chosen potential energy branch. In the pure prismatic loop picture the barrier is substantial, ranging from 8 eV, 2 eV, and 0.4 eV for separations Δx of 8 nm, 12 nm, and 20 nm, respectively. In contrast, the lowest PES branches have dramatically reduced barriers to trapping of 2 eV, 0.5 eV, and 0.1 eV, respectively, and as such may eventually be overcome by diffusion. In our earlier work based on a pure prismatic loop picture, where elastic interaction between the loops was described by the Foreman-Eshelby equation (Foreman and Eshelby, 1962; Barnes, 1963), the trapping barrier had to be artificially lowered to facilitate elastic confinement of loops, as otherwise no formation of loop rafts would occur (Dudarev et al., 2010).

We also note that in the limit of large separation *s*, only three PES branches form. The corresponding fundamental configurations of pairs of loops are shown in Fig. 2.5b, and their energy ordering is consistent with the separations Δx studied here.

This comparison demonstrates that the energy of interaction between prismatic loops



FIGURE 2.6: Comparison of energies of elastic interaction of two pure prismatic dislocation loops of radius $\rho = 4.09$ nm, obtained by exact integration (solid, blue) and computed in the dipole tensor approximation using the Foreman-Eshelby equation (Foreman and Eshelby, 1962; Barnes, 1963; Dudarev et al., 2010) (dashed, red). Allowing the loops to tilt, and thus to acquire a mixed character, reveals a complex potential energy surface (solid, grey). Plots A to D represent loop pairs with increasing separation Δx perpendicular to the glide cylinders.

is strongly affected by the internal degrees of freedom of the loops. Consequently, the competition between the elastic energy and the core energy plays a pivotal role in determining the landscape of binding energies of loops. This subtlety is neglected in any physical approximation where the dislocation loops are treated as being purely prismatic, or where they are treated as point-like objects defined only by their position in real space and involving no consideration of their internal degrees of freedom.

In what follows, we carry out stochastic dislocation dynamics simulations of interacting pairs of loops. The simulations start from large initial separations Δx and s at 200 K in an attempt to emulate various elementary interactions observed in experiment, see Section 1, namely coalescence, repulsion, and mutual elastic confinement of interacting loops.

Case A: Coalescence of dislocation loops

The coalescence of dislocation loops was observed using TEM and was found to involve loops of comparable size (Arakawa et al., 2011), with diameters larger than 4 nm. To match experimental observations, two pure prismatic hexagonal $\langle 111 \rangle$ loops with $\rho = 4.5$ nm are introduced in a simulation cell with separations of $\Delta x = 8$ nm and s = 5 nm, yielding a mutually attractive elastic force, see Fig 2.6. Note that the glide cylinders of the loops overlap slightly. Sequential snapshots taken during simulations are shown in Fig. 2.7a. The loops coalesce into a larger prismatic loop, with small debris released and ejected by a strong repulsive elastic force.

The corresponding time evolution of the diffusion coefficient of the resulting large loop is shown in Fig. 2.7b. We observe that the diffusion coefficient becomes constant over the interval of a few nanosecond and converges to a notably smaller value than the diffusion coefficient of single loop with $\rho = 4.5$ nm. Using the $D_{\text{COP}} \propto 1/L$ scaling relation, the equivalent loop size of the loop produced by the coalescence of a pair of loops equals $\rho_{eq} \approx 7$ nm. This is consistent with an estimate of the equivalent loop size obtained by removing a quarter of each loop's circumference, leading to $\rho_{eq} \approx 3/2\rho$. While the relaxation volume of the loops is a conserved quantity, the length of the loop circumference is not; this example demonstrates clearly that the effective diffusivity of an ensemble of prismatic loops may reduce over time as a result of coalescence of loops.

Case B: Repulsion between the loops

An example of repulsive interaction between diffusing dislocation loops is obtained by placing the loops with separations of $\Delta x = 5 \text{ nm}$ and s = 7 nm, using three different initial configurations shown in Fig. 2.5b. Note that configuration 1 was placed at a separation of s = 12 nm, as its corresponding PES branch vanishes at closer separation. Fig. 2.8 shows the evolution of the corresponding interaction energies during the simulation performed without stochastic forces (T = 0 K) and with stochastic forces (T = 200 K) included, in comparison with the theoretical prediction derived from examining the corresponding potential energy surface.



b) diffusion coefficient as a function of time

FIGURE 2.7: (a) Shapshots taken from stochastic dislocation dynamics simulations of a loop coalescence reaction, for the initial loop-pair separations of $\Delta x = 8 \text{ nm}$ and s = 5 nm, viewed at an angle from the $-\hat{y}$ direction. Note the occurrence of ejection of debris during loop coalescence. b) Plot of the effective diffusion coefficient as a function of time. The dotted line is a reference value computed for a single loop with size $\rho = 4.5 \text{ nm}$.

As expected for repulsive configurations, we find that the distance between the loops gradually increases over the interval of time spanned by the simulation. Inspection of the loop-pair configuration shows that the cold (T = 0) systems retain their initial orientation of the habit plane, which is consistent with the energy trajectories propagating along the distinct PES branches. On the other hand, the trajectories of the heated system (T = 200 K) soon start overlapping, starting from $s \approx 20 \text{ nm}$, eventually becoming indistinguishable. The stochastic force supplies additional thermal energy to the loops, which is evidently sufficient to overcome the energy barrier between the different PES branches, enabling the loops to rotate and thus oscillate between various tilting configurations.

Case C: Elastic confinement of loops

Prismatic loops may exhibit strong elastic attraction and form an elastically confined configuration as seen in Fig. 2.6. Depending on loop size and loop separation, the binding energy can vary from meVs to eVs, potentially surpassing the binding energy of dislocations to substitutional defects. Therefore it can be reasoned that elastic confinement of loops represents the key step leading to the stabilization of experimentally observed rafts of dislocation loops.

We adopt the initial setup corresponding to $\Delta x = 12 \text{ nm}$ and s = 12 nm, for which the pair of loops exhibit mutual attraction. As in the repulsive case investigated above, the simulations were run for three initial loop configurations shown in Fig. 2.5b, corresponding to distinct branches of the potential energy surface. The evolution of the energy of interaction between the two loops as a function of their separation in comparison with the idealized PES is shown in Fig. 2.9.

In the absence of stochastic forces, the two-loop system is hindered from reaching the lowest energy state because it is unable to overcome the energy barrier associated with the rotation of the loop habit planes. In contrast, the addition of stochastic forces supplies the loops with additional energy, enabling the system to explore the potential energy landscape more freely to the point where it even oscillates around the global energy minimum. As in the loop repulsion case investigated above, the interaction energy derived using simulations involving elevated temperature is found to be shifted upwards by about 1.5 eV compared to the PES, as the Langevin thermostat adds additional energy to the system.

The COP trajectories of the two loops corresponding to conf. 1 state are shown in Fig. 2.10. After a brief initial relaxation time, the loops become mutually trapped in their relative frame by attractive elastic interaction, with their COP trajectories becoming strongly spatially correlated. The loop separation distance in the elastically confined state fluctuates around the global potential energy minimum as a result of the effect of stochastic force, in agreement with experimental observations and simulations reported in Figs. 3-5 of Ref. (Dudarev et al., 2010). Interestingly, the simulated trajectories suggest that the bound two loops oscillate on a ~ 0.5 ns time-scale, thus evolving significantly slower than the tilt angle of the isolated loop, see Fig. 2.3.



FIGURE 2.8: Dislocation dynamics simulation of two prismatic loops in a repulsive arrangement without (A) and with stochastic forces at T = 200 K (B) included. The initial loop configurations (conf.) are taken from Fig. 2.5. Trajectories in (B) are shifted down by an estimated amount of additional thermal energy supplied by the thermostat W^{th} for better comparison. In the absence of stochastic forces the system of two loops moves along the PES branches, see conf. 2 and conf. 3 in (A). On the other hand, the trajectories of the heated system eventually become indistinguishable, oscillating between various tilting configurations.



FIGURE 2.9: Dislocation dynamics simulation of a pair of prismatic loops in an attractive arrangement without (A) and with stochastic forces at T = 200 K (B) included. The initial configurations (conf.) of loops are taken from Fig. 2.5. Trajectories in (B) are shifted down by an estimated amount of additional thermal energy supplied by the thermostat W^{th} for better comparison. In the absence of stochastic forces, the loop-pair is stuck in metastable configurations. In contrast, the heated system escapes from the metastable state, instead fluctuating around the global minimum.

4 The lifetime of elastically confined loop configurations

In Section 3.2 above, we have explored the three types of fundamental reactions between prismatic dislocation loops. These reactions, namely loop coalescence, repulsion and mutual elastic trapping or confinement, have all been modelled using stochastic dislocation dynamics at 200 K. The simulations enable comparison with models developed earlier for modeling the thermal evolution of multiple loops, which involve the dipole approximation (Dudarev et al., 2014) and treat the loops as point objects, assuming that they remain purely prismatic over the duration of the simulation. In this paper we show that the internal degrees of freedom significantly influence the nature of interaction between the loops, with potentially significant implications for the lifetime of elastically confined loop configurations. We now analyze this effect quantitatively.

Introducing the probability density P(s,t) of finding the two loops at separation s at time t, the equation of motion for this probability density, see Appendix B, can be expressed as a Fokker-Planck equation (Risken, 1996; Melnikov, 1991; Felderhof, 2009)

$$\frac{\partial P(s,t)}{\partial t} = -\frac{\partial J(s,t)}{\partial s},\tag{2.22}$$

where J is the flux of the probability density

$$J(s,t) = -\frac{2}{\beta BL} e^{-\beta V(s)} \frac{\partial}{\partial s} \left(e^{\beta V(s)} P(s,t) \right), \qquad (2.23)$$

where $\beta = 1/(k_BT)$ and V(s) refers to a branch of the potential energy surface. It is sufficient to consider the $s \in [0, +\infty)$ interval of variation of *s* as the potential energy surface is symmetric. In the following discussion we assume that the potential energy



FIGURE 2.10: *z*-coordinates of centers of elastically confined loops plotted versus simulation time. The initial position of the loops corresponds to conf. 1.

surface includes a confined state that transforms, over an energy barrier, into an unbound state at large separation *s*. While this assumption is valid for a pair of loops, caution needs to be taken in densely populated microstructures, as the potential energy can be strongly distorted by the elastic field of other defects.

Consider now the pair of loops at an energy minimum at s_{\min} . At equilibrium steady state the flux vanishes, J = 0, leading to the probability acquiring the form of the Gibbs distribution $P(s) \sim \exp(-\beta V(s))$. Similarly, the escape process from the energy minimum at s_{\min} to a very far separation along the glide direction $s_{\text{far}} \gg s_{\min}$ can be considered to proceed slow enough to preserve the steady-state, leading to a constant flux $J = J_0$. The steady-state flux is found by solving Eq. (2.23) for the derivative and subsequently integrating from s_{\min} to s_{far} , namely

$$\left[e^{\beta V(s)}P(s)\right]_{s_{\min}}^{s_{\max}} = -\frac{J_0\beta BL}{2} \int_{s_{\min}}^{s_{\max}} \mathrm{d}s \ e^{-\beta V(s)}.$$
(2.24)

Using $P(s_{\min}) \gg P(s_{far})$, the escape flux can be found as

$$J_0 \approx \frac{2}{\beta BL} \frac{e^{\beta V(s_{\min})} P(s_{\min})}{\int_{s_{\min}}^{s_{\max}} ds \ e^{\beta V(s)}}.$$
(2.25)

Assuming that the probability density decays rapidly outside the potential well associated with the energy minimum, the probability p of finding the pair of loops in an elastically confined state is derived by integration over the well width $\pm \delta s$, using the method of steepest descent

$$p = \int_{s_{\min}-\delta s}^{s_{\min}+\delta s} ds P(s)$$

= $P(s_{\min}) \int_{s_{\min}-\delta s}^{s_{\min}+\delta s} ds e^{-\beta(V(s_{\min})-V(s))}$
 $\approx \frac{P(s_{\min})}{2} \int_{-\infty}^{+\infty} ds e^{-\beta V''(s_{\min})s^2/2}$
= $\frac{P(s_{\min})}{2} \left(\frac{2\pi}{\beta V''(s_{\min})}\right)^{1/2}$ (2.26)

where $V''(s_{\min})$ is the second derivative of V(s) evaluated at the stationary point s_{\min} . Similarly, the integral term in Eq. (2.25) peaks at the point s_{\max} corresponding to the maximum barrier height. Applying the same approach as in Eq. (2.26), the escape rate Γ can be finally expressed as

$$\Gamma \equiv \frac{J_0}{p} = \frac{\left(V''(s_{\min}) \left|V''(s_{\max})\right|\right)^{1/2}}{2\pi BL} e^{-\beta \Delta V}$$
(2.27)

where $\Delta V = V(s_{\text{max}}) - V(s_{\text{min}})$ is the energy barrier that the pair of loops has to overcome in order to separate. The inverse of the escape rate equals the lifetime of the confined state

TABLE 2.2: The lifetime of an elastically confined pair of dislocation loops computed for some selected loop radii ρ and temperatures *T* assuming the separation between the loops in a plane perpendicular to their glide cylinders of $\Delta x = 12$ nm. Three distinct configurations of pairs of loops are considered.

Conditions	Pure prismatic	Lowest PES	30° fixed tilt
$\rho = 4.5 \mathrm{nm}, T = 200 \mathrm{K}$	$\sim 10^{259} { m yr}$	$\sim 10^{258} \mathrm{\ yr}$	$+\infty$
$\rho = 4.5 \mathrm{nm}, T = 600 \mathrm{K}$	$\sim 10^{75} { m yr}$	$\sim 10^{75}~{\rm yr}$	$\sim 10^{117} { m yr}$
$\rho = 2.0 \text{nm}, T = 200 \text{K}$	4 s	18 min	3 yr
$\rho = 2.0 \mathrm{nm}, T = 300 \mathrm{K}$	5 µs	0.3 s	5 min
$\rho = 2.0 \text{nm}, T = 400 \text{K}$	0.2 ms	6 ms	0.5 s
$\rho = 2.0 \text{nm}, T = 500 \text{K}$	0.02 ms	0.5 ms	10 ms
$\rho = 2.0 \mathrm{nm}, T = 600 \mathrm{K}$	0.005 ms	0.1 ms	0.8 ms

of the loops. Under these conditions, a small variation of ΔV can significantly affect the lifetime.

Consider now the choice of the potential branch V(s). We use three different tilting configurations to investigate the effect of internal degrees of freedom on the confinement life-time. First, the pure prismatic pair of loops is a reference configuration to models involving no internal degrees of freedom. Next, the freely tilting loop-pair is represented by the lowest energy curve of the PES. Finally, the tilting of each loop is fixed ad-hoc at an angle of 30° each (unfavourable in energy, see conf. 1 in Fig. 2.5b), in an attempt to mimic the habit plane locking observed in molecular dynamics. The corresponding lifetimes of elastically confined loop configurations are listed in Tab. 2.2 for circular loops with $\rho = 4.09$ nm and $\rho = 1.8$ nm, which are equivalent to hexagonal loops with $\rho = 4.5$ nm and $\rho = 2$ nm. In either case the separation between the two loops in the plane perpendicular to the glide cylinders is chosen as $\Delta x = 12$ nm.

Tab. 2.2 shows that the lifetime of loops depends strongly on the loop size and temperature. For $\rho=4.5\,\text{nm}$ the pair of loops is effectively unable to escape from the elastically confined state, as the lifetime is dominated by the escape barrier of $\approx 10 \text{eV}$. On the other hand, the lifetime of an elastically confined configuration involving smaller loops $\rho=2\,\text{nm}$ is comparable with experimental timescales even at low temperatures.

The specific form of configuration of interacting dislocation loops is found to have a most significant effect on its lifetime. An approximation where the loops are treated as pure prismatic objects underestimates the escape time in comparison with the case of freely rotating loops by several orders of magnitude. In contrast to that, the pair of loop with the orientation of their habit planes fixed at 30° has a significantly longer life-time in comparison with a freely rotating pair of loops, and it only breaks apart at relatively high temperatures. This offers a possible explanation for why the experimentally observed rafts of loops remain stable over an appreciable temperature range, while a simple estimate based on the purely prismatic picture of interacting loops predicts much shorter lifetimes (Dudarev et al., 2010). The loop habit plane reorientation not only changes the barrier that the system needs to overcome in order to escape, but most importantly it strongly lowers the curvature of the potential energy barrier, see Fig. 2.6, hence further increasing the lifetime of an elastically confined configuration by several orders of magnitude.

5 Conclusion

The stochastic motion of prismatic dislocation loops diffusing in the glide direction is successfully simulated using dislocation dynamics that also includes the stochastic thermal forces treated using the Langevin equation formalism. The dependence of the diffusion coefficient of a dislocation loop on temperature is consistent with molecular dynamics simulations.

Reactions involving interacting dislocation loops, including loop coalescence, repulsion and the formation of an elastically confined pairs of loops, are well reproduced using the stochastic dislocation dynamics framework proposed above. The internal degrees of freedom of interacting loops result in the formation of complex potential energy landscape of states with distinctly tilted loop habit planes, separated by potential barriers. The addition of thermal energy through stochastic Langevin forces acting on dislocation lines enables interacting loops to switch between the tilted configurations, allowing the system to explore the entire energy landscape of excited states.

In comparison to the purely prismatic case of interacting loops first explored by Foreman and Eshelby (1962), the reorientation of the habit plane of interacting loops is found to strongly affect the rates of reactions resulting in the elastic confinement of loops. For one, the potential barrier for the elastic trapping a loop approaching another loop from a distance is strongly reduced, making it much more likely for loops to form elastically trapped configurations. Secondly, the lifetime of the elastically confined state increases by several orders of magnitude, bringing the estimated lifetime into broad agreement with experimental observations. The habit plane reorientation effect highlights the pivotal significance of including internal degrees of freedom of loops in the treatment of microstructural evolution, to achieve a physically consistent description of dynamics of complex dislocation microstructures.

A Potential energy surface of the loop-pair

Given a vector z containing all the node positions, we define a set of local energy minima that depend parametrically on the distance between the loops

$$V_{\mathcal{S}}(s) = \{ W^{tot}(\boldsymbol{z}) \mid \boldsymbol{z} \in \mathcal{Z} \text{ is a local minimum} \},$$
(A.1)

where

$$Z = \{ z \mid z_{\text{COP}}^{(2)} - z_{\text{COP}}^{(1)} = s \}$$
(A.2)

refers to the set of nodal positions for which the separation between the loops is *s*. In other words, the loop separation is held constant, whereas the remaining internal degrees of freedom are varied to find local potential energy minima.

The potential energy surfaces defined by Eqs. (A.1)-(A.2) are found by the numerical minimization of energy of a simplified system of two loops. The internal degrees of freedom are reduced to tilting modes only, leading to the following parameterization of the dislocation loop:

$$\boldsymbol{r}(\boldsymbol{\psi}) = \begin{pmatrix} \rho \cos \boldsymbol{\psi} \\ \rho \sin \boldsymbol{\psi} \\ u \sin \boldsymbol{\psi} + v \cos \boldsymbol{\psi} \end{pmatrix}, \qquad (A.3)$$

where $\psi \in [0, 2\pi)$ is the parameterization variable, and $u \in \mathbb{R}$ and $v \in \mathbb{R}$ are tilting amplitudes. The normal vector of the parameterization is independent of ψ and is free to point in any direction, while the loop relaxation volume is constant as $\Omega_{rel} = \mathbf{A} \cdot \mathbf{b} = \pi \rho^2 \mathbf{b}$. Thus the loop habit plane may tilt freely within the glide cylinder. The above parameterization may also be used to include tilting in the dipole-tensor approximation (Dudarev and Sutton, 2017), though for carrying out a dynamic simulation one would also need an approximate analytic expression for the self-energy of a mixed ellipsoidal loop. Some expressions suitable for this purpose are already available in literature (Wolfer et al., 2004; Chu et al., 2011), but they are relatively limited in comparison with the general case addressed here.

The total potential energy of interacting loops is computed using the non-singular de Wit formula (Cai et al., 2006), including the line tension core energy (2.3). The energy has multiple stationary points at a given separation *s*, which are not trivially identified. Here the total energy was minimized over tilt amplitudes of both loops $\{u^{(1)}, v^{(1)}, u^{(2)}, v^{(2)}\}$ using the BFGS (Nocedal and Wright, 2006) implementation in SCIPY (Jones et al., 2001) for a broad range of initial tilt configurations. While this approach does not consistently identify all the stationary points, it still gives a qualitative overview of the potential energy landscape.

All the energy minima identified in this way are shown in Fig. 2.6. Multiple potential energy branches belonging to distinct tilt configurations are found. Note that transitions at a crossing may involve a significant change in tilting, and thus would involve a transition over a large energy barrier.

B Langevin equation of motion for the loop-loop separation

Assuming that the relaxation of internal loop degrees of freedom occurs on a much shorter time-scale than the COP diffusion, the adiabatic equation of motion for the individual loop COP is derived from the two equations of motion for the loops

$$B\dot{z}_{COP}^{(1)} = -\frac{1}{L^{(1)}} \frac{\partial V(s)}{\partial z_{COP}^{(1)}} + F_s^{(1)}$$

$$B\dot{z}_{COP}^{(2)} = -\frac{1}{L^{(2)}} \frac{\partial V(s)}{\partial z_{COP}^{(2)}} + F_s^{(2)},$$
(B.1)

where $V \in V_S$ is a branch of the PES, and the total stochastic force $F_s^{(i)}$ with strength $\sigma_{COP}^{(i)}$ acting on loop *i* is derived following Section 2 using

$$\left\langle F_s^{(i)}(t)F_s^{(i)}(t')\right\rangle = \frac{\sigma_s^2}{L^{(i)}}\delta(t-t'),\tag{B.2}$$

leading to $\sigma_{\text{COP}}^{(i)} = \sigma_s / \sqrt{L^{(i)}}$. The total energy derivative is evaluated using the chain rule with $s = z_{\text{COP}}^{(2)} - z_{\text{COP}}^{(1)}$, and the two equations of motion (B.1) are subtracted to yield

$$B\dot{s} = -V'(s)\left(\frac{1}{L^{(2)}} + \frac{1}{L^{(1)}}\right) + F_s^{(2)} - F_s^{(1)}.$$
(B.3)

The equation of motion (B.3) simplifies further for the case $L^{(1)} = L^{(2)} = L$:

$$BL\dot{s} = -2V'(s) + F_s, \tag{B.4}$$

where F_s is the net stochastic force with standard deviation $\sigma = \sigma_s \sqrt{2L}$, following the sum theorem of Gaussian distributed variables. Note that the expectation value of the loop velocity over independent trajectories is temperature-independent as the stochastic force has zero mean:

$$\langle s \rangle = -\frac{2}{BL} V'(s). \tag{B.5}$$

Chapter 3

Cross-slip and loop-induced stress field effects on dislocation/loop interactions

This chapter is reproduced from:

Yang Li, Christian Robertson, Malik Shukeir, Laurent Dupuy (2018). Screw dislocation interaction with irradiation defect-loops in iron: evolution of cross-slip effect using dislocation dynamics simulations. Modelling and Simulation in Materials Science and Engineering, 26, 055009.

Yang Li, Christian Robertson, Malik Shukeir, Laurent Dupuy (2019). Screw dislocation interaction with irradiation defect-loops in iron: loop-induced stress field effect using dislocation dynamics simulations. Nuclear Instruments and Methods in Physics Research Section B, 458, 137.

Apart from elastic interactions of prismatic loops themselves as presented in Chapter 2, the dislocation networks strongly interact with these loops locally, which is responsible for the mechanical changes of irradiated materials such as hardening. In the present chapter, we perform the elementary dislocation/loop interactions in α -iron, with a particular attention on the examination of the cross-slip effect, by adopting a specific initial configuration associated with a screw dislocation glide plane change. Moreover, dislocation/loop simulation cases are systematically compared to equivalent dislocation/facet simulation cases, for the purpose of evaluating the separate contribution of the loop-induced stress on such interactions.

1 Introduction

Ferritic α -iron steels are widely used as structural nuclear materials, thereby subjected to neutron irradiation-induced degradation, including hardening and embrittlement (Bloom, 1998; Matijasevic et al., 2008; Baluc et al., 2007; Matijasevic et al., 2009). These detrimental evolutions are concurrent with and generally ascribed to the gradual accumulation of dispersed defect cluster populations, in the form of dislocation loops as discussed in Chapter 1. The defect dispersion characteristics, size and number density, depend on many different factors such as the irradiation temperature, cumulated dose and the material chemical composition (Nikolaev et al., 2002; Klueh et al., 2000; Victoria et al., 2000). Mobile dislocations generated during post-irradiation straining strongly interact with these loop/defect populations (Zinkle and Matsukawa, 2004; Masters, 1965; Byun and Hashimoto, 2006; Robach et al., 2003). At the grain scale, plastic strain spreading takes the form of wavy shear bands, controlling the subsequent stress-strain and fracture toughness responses (Wei et al., 2002; Odette et al., 2002; Chaussidon et al., 2010, 2008). Understanding the shear-band scale plasticity mechanisms is thus a crucial factor, in the management of nuclear structural material lifetime.

Dislocation/loop interactions have been recently investigated using atomistic Molecular Dynamics (MD) (Liu and Biner, 2008; Terentyev et al., 2010, 2008) or mesoscopic Dislocation Dynamics (DD) simulations (Shi et al., 2015; Greer et al., 2008; Drouet et al., 2014, 2016). These studies usually assume periodic boundary conditions, i.e. infinitely long mobile dislocations. Shear band development also involves the ubiquitous cross-slip mechanism, which possibly have a strong influence on the dislocation/loop interaction, with finite length (screw) dislocations (Shin et al., 2003; Kelly and Nicholson, 1971). Cross-slip is a time-dependent, stochastic phenomenon (Chaussidon et al., 2006; Püschl, 2002; Kelly et al., 2012; Bulatov and Cai, 2006) and for this reason, its specific contribution to the effective radiation-induced loop strength has not yet been measured or evaluated. Loop interaction strength assessment is attempted hereinafter, by means of DD simulations. This technique allows implementing a specific initial configuration, associated with a (screw) dislocation glide plane change, due to a single and well defined cross-slip event. That initial configuration is called a "composite dislocation source" (please refer to Fig. 3.1), which has been developed based on TEM observation of crossslip activity, in post-strained ferritic steel (Robertson and Meslin, 2011; Robertson et al., 2007). Such evaluation is generally not accessible to any other known investigation method, including experiments. For instance, crystal plasticity cannot treat cross-slip at the scale of individual dislocation/defect interaction, unless informed by other, lower scale simulation methods. The typical time step of atomistic (molecular dynamics) simulations is generally too brief however, to generate a composite source configuration within a reasonable simulation timeframe.

The following investigation approach is therefore adopted, based on the simulation method and setups as described in Section 2. Simulations using periodic boundary conditions (without pining points) are carried out first, as a benchmarking case (Section 3.1.1: $[1\bar{1}1]$ loop case; Section 3.2.1: [111] loop case). These results allow validating the adopted simulation parameters and setup, by comparison with well-established MD simulation results. The role of cross-slip is evaluated next, using DD simulations with "composite dislocation" sources. The results are compared with the preliminary case results : Section 3.1.2: $[1\bar{1}1]$ loop case; Section 3.2.2: [111] loop case.

In addition, this work is also devoted to evaluating the specific contribution of the loop-induced stress field on such dislocation/loop interaction with respect to dislocation mobility, in presence of cross-slip mechanism and under room temperature straining conditions. This effect is highlighted by systematic comparison between simulation setups where the loops have been replaced by hard impenetrable platelets (or facets), without any associated elastic stress field. Interactions of composite source with $[1\bar{1}1]$ and [111] facets are therefore examined and compared with the dislocation/loop cases, in Sections 4.1 and 4.2 respectively. This work focused on pure Fe, taken as a model ferritic material, for which all the material parameters are well-characterized (Alshits and Indenbom, 1986; Urabe and Weertman, 1975).

2 Simulation method and setups

2.1 Dislocation Dynamics simulation setup and model : benchmarking case

All DD simulations results presented in this work are performed using a 3D nodal code called NUMODIS (e.g. Shi et al. (2015) and Drouet et al. (2014, 2016)), developed in CEA. The dislocation lines are described by a series of inter-connected nodes. Computation of the internal elastic stress and corresponding nodal force is carried out within the frame of the non-singular continuum elastic theory (Cai et al., 2006). The stress at any arbitrary point is due to the total stress field:

$$\underline{\underline{\sigma}} = \underline{\underline{\sigma}}^{app} + \underline{\underline{\sigma}}^{int} \tag{3.1}$$

including the applied $\underline{\underline{\sigma}}^{app}$ and internal $\underline{\underline{\sigma}}^{int}$ stress field contributions. The force per unit length on the connected dislocation nodes is given by Peach-Koehler formula:

$$\boldsymbol{f}^{PK} = (\boldsymbol{\underline{\sigma}} \cdot \boldsymbol{b}) \times \boldsymbol{\xi} \tag{3.2}$$

where b is the dislocation Burgers vector and ξ is the local line direction. The PK force, together with the contribution associated with the dislocation core energy is converted into nodal force by a weighting shape function. The present study is restricted to room temperature straining conditions, where screw dislocation velocity is a quasi linear function of the effective shear stress, through an effective drag coefficient B (Alshits and Indenbom, 1986; Urabe and Weertman, 1975; Po et al., 2016), which characterizes the phonon scattering effect,

$$\underline{B}\boldsymbol{v} = \boldsymbol{f}^{tot} \tag{3.3}$$

Please note that unlike Chapter 2, only the elastic portion of the driving force is considered in the present work. The material parameters corresponding to pure Fe are listed in Tab. 3.1 below.

As a first investigation step, preliminary DD simulation results are benchmarked by comparison with MD simulations using a similar configuration as shown in Fig. 3.1. The

parameter	symbol	value
Burgers vector	b	2.47 Å
Shear modulus	μ	63 GPa
Poisson's ratio	ν	0.43
Drag coefficient	В	0.08 MPa · ns
Core radius	а	2.5 Å

TABLE 3.1: Pure Fe materials parameters at 300 K. (Shi et al., 2015; Shukeir, 2019; Alshits and Indenbom, 1986; Urabe and Weertman, 1975)

simulated crystal orientations as X, Y and Z axis are parallel to the $[\bar{1}\bar{1}2]$, $[1\bar{1}0]$ and [111] directions, respectively. The DD simulated volume dimensions are : $L_x = 400$ nm, $L_y = 300$ nm and $L_z = 400$ nm, which is consistent with the shear bands thickness observed in post-irradiated materials (Odette et al., 2002; Gururaj et al., 2015a). One screw dislocation source, with its Burgers vector **b** parallel to the Z direction, is placed at the center of the simulation volume. The total length of the source is L, which is comparable to the dimensions of the simulation volume. In all the cases, one SIA loop/obstacle is placed at a short distance from the mobile dislocation source, as discussed in the next section and shown in Fig. 3.1 below.

The complementary simulation parameters and slip systems common to all the simulation cases are listed Tab. 3.2:

TABLE 3.2: Simulation parameters.

Time step	Discretization length	Primary slip system	Cross-slip system
50 fs	10 Å	$(1\bar{1}0)[111]$	$(10\bar{1})[111]$

2.2 Dislocation Dynamics simulation setup and model: various dislocation source cases

A composite dislocation source configuration is shown in Fig. 3.2 with the initial line direction from node A to node B. The left-hand part of Fig. 3.2 defines the total source length L and source-loop initial stand-off distances L_1, L_2 . The implemented loop is placed at distance L_1 from segment BC and has a diameter D = 6 nm. The center of the loop is coplanar with the dislocation line and $L_2 = L/4$ from point B (at the center of segment BC). The chosen defect position (typically 15 nm or less) ensures early contact between the dislocation and the immobile defect/loop. Small variations of L_1 has a minor effect on the results since $L_1 \ll L$, while the influence of L_2 will be discussed in Section 3. The right-hand part of Fig. 3.2 shows the two segments AC and BC forming the composite source. Segment AC is L_{cs} long which glides in the cross-slip system and segment BC is L_p long and glides in the primary slip system. The loop information is same as former case with $L_2 = L_p/2$.



FIGURE 3.1: DD simulation volume adapted to dislocation-loop interaction investigation. (a) This configuration has no cross-slip arm and lead to coplanar dislocation/interaction. The highlighted primary slip plane contains a screw-type dislocation source. (b) The composite dislocation source consisting of a finite length pinned source with one arm BC gliding in the primary slip plane, connected to another arm AC gliding in the cross-slip plane. This finite length configuration is compatible with TEM observations post-irradiated, strained specimens (Robertson and Meslin, 2011). The simulated space dimensions and interface properties are explained in the main text.



FIGURE 3.2: Composite dislocation source configuration. Left-hand sketch: total source length *L* and definition of source-loop initial standoff distances L_1 , L_2 . Nodes A and B are fixed with the initial line direction **AB**. Right-hand sketch: Segment AC is L_{cs} long and glides in the cross-slip plane (101); segment BC is L_p long and glides in the primary slip plane (110).

In the current NUMODIS code, the twinning-anti-twinning asymmetry of BCC Fe is not implemented. The selected cross-slip plane $(10\overline{1})$ is in the twinning direction for information.

Nodes A and B are pinned, i.e. do not move during the simulation time similar to a Frank-Read source. Node C is the common point connecting the two segments gliding in different slip planes. For this reason, node C moves parallel to the initial direction of the dislocation line. If node C moves toward to node B, the length L_{cs} of segment AC increases and vice versa. It should be mentioned that the non-periodic boundary condition is used for all pinned configurations and the simulation is terminated whenever a dislocation node reaches one of the simulation volume boundaries.

2.3 Activation of the composite dislocation source: theoretical analysis

The total dislocation energy of the dislocation source in Fig. 3.2 configuration is the sum of the elastic and core contributions. In the non-singular continuum elastic theory, the elastic energy is given in Appendix Section of (Cai et al., 2006; Bulatov and Cai, 2006),

whereas the core energy per unit length is (Dupuy and Fivel, 2002):

$$e^{core} = \zeta^{core} \frac{\mu b^2}{4\pi (1-\nu)} (1-\nu \cos^2 \theta)$$
(3.4)

where $\zeta^{core} = 0.6$ is a correction coefficient and θ is the angle between the Burgers vector and the local tangent vector. The correction coefficient and core radius used in the nonsingular stress field calculations for screw dislocations are calibrated as explained (Shukeir, 2019). The total energy of the composite source is thus independent of the cross-slip segment length. In these conditions, there is no driving energy to either shrink or spread the added cross-slip segment, along the original dislocation line.

In absence of obstacle, segment AC and BC evolutions involve the one-dimensional displacement of the common node C. For segment AC gliding in the cross-slip plane, the core energy contribution to the force exerted on node C can thus be expressed as:

$$\boldsymbol{F}^{AC} = e^{core} \boldsymbol{T} + \frac{\mathrm{d}e^{core}}{\mathrm{d}\theta} \boldsymbol{N}$$
(3.5)

where T and N are the corresponding local tangent and normal vectors. Since node C moves parallel to the Burgers vector, projection of this force along the Z-axis yields:

$$\boldsymbol{F}^{AC} = \zeta^{core} \frac{\mu b^2}{4\pi (1-\nu)} (1 - 2\nu + \nu \cos^2 \theta_{AC}) \cos \theta_{AC}$$
(3.6)

where θ_{AC} is the angle between the Z-axis and the local tangent vector of segment AC at node C. The force from segment BC is given by a similar expression, so the total nodal force due to the core energy corresponds to:

$$\boldsymbol{F}^{C} = \zeta^{core} \frac{\mu b^{2}}{4\pi (1-\nu)} \left[(1-2\nu+\nu\cos^{2}\theta_{AC})\cos\theta_{AC} - (1-2\nu+\nu\cos^{2}\theta_{BC})\cos\theta_{BC} \right]$$
(3.7)

A positive force means that the length of segment AC is increasing at the expense of segment BC and vice-versa, for a negative force. It is worth to note that the core energy of a dislocation line is almost ~ 10% of its total energy. Therefore using the line tension model, the nodal force associated with the total energy can be also expressed in the form of Eq. (3.7), but with a correction coefficient $\zeta^{LT} \sim 10\zeta^{core}$. In this regard, Eq. (3.7) thus indicates that segment AC evolutions are qualitatively the same, that is depending on the motion of node C, regardless of the number of sub-segments (or obstacles) placed beyond node C (Gururaj, 2013). In the rest of this work, we therefore focus on the two segments composite sources, for simplicity.



FIGURE 3.3: Interaction between an infinite screw dislocation and a $[1\bar{1}1]$ dislocation loop. The screw dislocation glides in the direction of X-axis ($[\bar{1}12]$ direction). (From Shukeir 2019)

3 Effect of the cross-slip

3.1 Interaction with $[1\overline{1}1]$ loop

3.1.1 Interaction mechanism and obstacle strength: planar dislocation source

The implemented $[1\overline{1}1]$ hexagonal loops are composed by six edge segments belonging to the $(\overline{1}01)$, $(0\overline{1}\overline{1})$ and (110) planes, respectively.

DD simulation results obtained using periodic boundary conditions are compared with MD simulation results. In this case, controlled strain rate loading conditions (along YZ direction) are used, where the total strain rate $\dot{\epsilon}_{YZ} = 10^5 \text{ s}^{-1}$. Interaction with the screw dislocation changes the loop Burgers vector from $[1\bar{1}1]$ to $\boldsymbol{b} = [010]$, after the interaction is completed and the mobile dislocation breaks away from the loop as shown in Fig. 3.3.

The corresponding stress-strain evolutions are presented in Fig. 3.4. The interaction strength corresponding to this mechanism is $\tau_c = 0.4\mu b/(L-D)$, in good agreement with corresponding MD results (i.e. $\tau_c = 0.38\mu b/(L-D)$ from Liu and Biner (2008)). For more details regarding the infinite dislocation cases, please refer to Chapter 4 of Shukeir

(2019).



FIGURE 3.4: The stress-strain curves of $[1\overline{1}1]$ loop, [111] loop and $[1\overline{1}1]$ facet benchmarking cases (Fig. 3.1a), respectively.

The next simulation case is carried out using exactly the same strain rate as before, this time using a finite-length dislocation source (L = 300 nm), where nodes A and B are pinned (c.f. Fig. 3.2) and both segments AB and BC glide in the same primary slip plane (110). The resulting interaction mechanism is presented in Fig. 3.5. The screw dislocation is initially attracted by the loop and reacts with segment '2' (of the loop) to form a [010] junction (Fig. 3.5b), according to Frank's rule (1/2[111]- 1/2[111] = [010]). This particular reaction is embedded in the NUMODIS DD code, based on the interaction mechanism predicted by atomistic MD simulations, in the selected case studies (Terentyev et al., 2010, 2008). Thereafter, the new segments '3', '4' and the initial screw dislocation segments rearrange as shown in Fig. 3.5c (Case II) and 3.5d. At this stage, the initial loop has two distinct parts, with Burgers vectors b = [111] and b = [010]. During the final interaction stage (Figs. 3.5e, 3.5f), b = [010] of the junction segment returns to b = [111].

Fig. 3.5c highlights the effect of using periodic boundary condition (Case I) on the dislocation-loop reaction. In Case I, the radius of curvature of the interacting dislocation segment is maximal. At the time of contact, the incoming $b = [1\overline{1}1]$ screw arm can then easily adopt and keep its b = [010] orientation. The angle between the bowed-out dislocation segment and segment '3' is comparatively much larger (Case II). This condition lowers the attractive force between the incoming dislocation line and the remaining loop segments. The b = [010] junction segment cannot develop in this situation and usually collapses, after the interaction completion.

This configurational change also affects the effective loop interaction strength as shown


FIGURE 3.5: Interaction between a coplanar, pinned screw dislocation and a $[1\bar{1}1]$ dislocation loop. The screw dislocation glides in the direction of X-axis ($[\bar{1}12]$ direction). The dislocation-loop interaction proceeds from frame (a) to frame (f). Frame (c) highlights the configurational difference achieved between the periodic boundary condition (Case I) and the composite source (Case II), shortly after the dislocation-loop contact time (corresponding to frame (b)).

in Fig. 3.6 for different source cases. The critical loop strength evolution obtained from these simulations can be described using the following expression:

$$\tau_c = \tau_{eff} + \tau_{LT}^{etra} = \left(\alpha_{eff} + \frac{1}{\alpha_{LT}}\right) \frac{\mu b}{L - D}$$
(3.8)

where μ is the shear modulus (see Tab. 3.1), *b* is the magnitude of Burgers vector, $\alpha_{eff} = 0.4$ and $\alpha_{LT} = 0.42$. The correction term τ_{LT}^{etra} represents the extra line tension contribution associated with the difference in local dislocation curvature (see Fig. 3.5c), due to the pinning points of the finite length source (Foreman, 1967; Hull and Bacon, 2001). It is important to note that the screw dislocation is systematically released before adopting a semi-circular bowed-out configuration, while the loop is mostly immobile (with respect to the dislocation). As a result, the line tension correction and the loop strength τ_c (~150 MPa) are both nearly constant, regardless of L_2 (or L_p), within the [L/6, L/2] range (see also Fig. 3.10 data, for different L_p and therefore, L_2 values).



FIGURE 3.6: $[1\bar{1}1]$ loop strength evolution with reciprocal of dislocation source length 1/(L-D). Infinite source in presence of periodic boundary conditions : DD simulation results closely match the MD simulations results. A finite length source includes pining points, inducing dislocation curvature and hence, additional line tension stress τ_{LT}^{etra} . Eq. (3.8) thus illustrates the consistency of our DD model with the well-known continuum theory and MD simulation results.

3.1.2 Interaction mechanism and effective obstacle strength: composite dislocation source

The composite dislocation source case is systematically investigated with four different simulation sets, using double constant shear stress (τ_p , τ_{cs}) conditions and finite L_p

long dislocation segments (see Tab. 3.3 and caption), gliding in the primary slip plane. The applied stress tensor $\underline{\sigma}^{app}$ in local reference is given as

$$\begin{pmatrix} 0 & 0 & 0.577\tau_p - 1.155\tau_{cs} \\ 0 & 0 & \tau_p \\ 0.577\tau_p - 1.155\tau_{cs} & \tau_p & 0 \end{pmatrix}$$

The shear stress in the cross-slip plane thus equals $\left(\underline{\underline{\sigma}}^{app} \cdot \hat{n}_{cs}\right) \cdot \hat{b} = \tau_{cs}$, where \hat{n}_{cs} is the unit normal vector of the cross-slip plane and \hat{b} is the unit Burgers vector in the local reference. Similarly, the shear stress in the primary slip plane is τ_p .

TABLE 3.3: Simulation sets including a composite dislocation source, where the length is in nm and the stress is in MPa. Each set corresponds to several different simulations, where (τ_p, τ_{cs}) vary by $\tau_{p,inc}$ and $\tau_{cs,inc}$ steps of 20 MPa. The selected τ_{min} and τ_{max} values are not arbitrary: τ_{min} exceeds the critical source activation stress, which ensures that the mobile dislocation moves towards the immobile loop; whereas τ_{max} exceeds the dislocation/loop breakaway stress, which ensures finding the critical interaction stress, for the different simulation setups.

		L_p	$\tau_{p,\min}$	$\tau_{p,\max}$	$\tau_{p,inc}$	$\tau_{cs,\min}$	$\tau_{cs,max}$	$\tau_{cs,inc}$
Set 1	300	250	100	200	20	100	200	20
Set 2	300	200	100	200	20	100	200	20
Set 3	300	150	100	200	20	100	200	20
Set 4	300	100	100	200	20	100	200	20

Each set is tested for different τ_{cs} levels acting on segment AC in the cross-slip plane and varying from ($\tau_{cs,\min} : \tau_{cs,\max}$) and likewise, τ_p levels acting on segment BC in the primary slip plane varies from ($\tau_{p,\min} : \tau_{p,\max}$). Each simulation case is carried out up to a specific simulation time, t_{\max} (typically, several nano-seconds) under a specific loading combination (τ_p , τ_{cs}). Once the dislocation reaches the simulation volume boundary or t = t_{\max} a new combination (τ_p , τ_{cs}) is generated according to the selected stress increment. The initial loading stress is set to 100 MPa (close to the obstacle strength reported in Section 3.1.1), so segment BC (gliding in primary slip plane) contacts the obstacle at an early stage of each simulated case.

As L_p for set 1 and set 2 is much larger than L_{cs} , they perform the similar behaviour to the planar dislocation configuration. One example of set 2 under loading conditions $\tau_p = \tau_{cs} = 120$ MPa is shown in Fig. 3.7. It is seen that segment BC glide into primary slip plan and then forms [010] junction with the loop while the node C moves towards the node A. Finally the dislocation source is blocked by the loop since τ_p is smaller than the obstacle strength. Please also note that one segment of the SIA loop belongs to the plane (110), which is perpendicular to the screw dislocation glide plane (110). This implies that this segment is sessile under the external applied stress.

One typical dislocation-loop interaction case is presented in Fig. 3.8, for loading conditions $\tau_p = \tau_{cs} = 120$ MPa of set 3. Segment BC interacts with the obstacle in Fig. 3.8b



FIGURE 3.7: Interaction between a composite dislocation source and a $[1\bar{1}1]$ loop. The source length $L_{cs} = 100$ nm for $\tau_p = \tau_{cs} = 120$ MPa. The screw dislocation segment BC glides in the X direction ($[\bar{1}12]$ direction).

and a [010] junction is formed at the point of contact. Segment BC is then blocked since the resolved shear stress τ_p is lower than the critical obstacle strength (from Fig. 3.6 : $\tau_c = \tau_{total} = \tau_{eff} + \tau_{LT}^{extra} \approx 150$ MPa). Meanwhile, segment AC propagates in the crossslip plane and its length L_{cs} increases as node C moves along the line direction towards node B (Fig. 3.8c). As node C contacts with the loop/obstacle, a mutual attraction occurs between segments AC and BC then segment BC gets past the loop. Soon after, the whole dislocation source is transferred into the cross-slip plane (Fig. 3.8d). The loop is released at this time, while its Burgers vector returns to [111].

The Z-coordinate of node C (see Fig. 3.8) moves as described in Fig. 3.9. During the early stages of the interaction, node C moves towards node B and hence, the cross-slip segment length L_{cs} gradually increases with time. After ~ 0.5 ns, segment BC is trapped by the loop and a plateau in the strain level was observed, accordingly. As segment AC continues to glide in the cross-slip plane, segment BC then starts changing its glide plane and node C resumes gliding toward the point B until $L = L_{cs}$. As node C meets with node B, the initial source is entirely transferred in the cross-slip plane, which generates a marked strain rate jump, after ~ 1 ns.

Simulation results associated with Tab. 3.3 cases are presented in Fig. 3.10 in the form of triplet number series (τ_p , τ_{cs} , S). The S = 0 (deep green) case indicates that the source is blocked by the obstacle; the S = 1 (purple) case indicates the source overcomes the defect while gliding in the primary slip pane; the S = 2 (white) case indicates



FIGURE 3.8: Interaction between a composite dislocation source and a $[1\bar{1}1]$ loop. The source length $L_{cs} = 150$ nm for $\tau_p = \tau_{cs} = 120$ MPa. The mobile screw dislocation segment BC glides in the X direction ($[\bar{1}\bar{1}2]$ direction). The dislocation-loop interaction proceeds from frame (a) through frame (d). Details regarding the interaction mechanism are provided in the main text.



FIGURE 3.9: The total strain and the corresponding node C position evolutions with the simulation time, for the $L_{cs} = 150$ nm and $\tau_p = \tau_{cs} = 120$ MPa case study. The initial position of node C corresponds to coordinate Z = 0.

the source overcomes the defect while gliding in the cross-slip plane (as in Fig. 3.8). Fig. 3.10 shows that a screw dislocation can directly cut through the obstacle provided $\tau_p > 150$ MPa which is consistent with Fig. 3.6 results. Obstacle by-passing occurs if $\tau_{cs} > \tau_{critical}(L_p)$ and $\tau_{cs} \ge \tau_p$ where $\tau_{critical}(L_p) = 120$ MPa if $L_p = 150$ nm; while $L_p > 150$ nm induces higher $\tau_{critical}(L_p)$. It should be noted that $\tau_{critical}(L_p = 150$ nm) is lower than $\tau_{critical}(L_p = 300$ nm) in absence of cross-slipped segment AC, i.e. 120 MPa instead of 150 MPa.



FIGURE 3.10: Dislocation reaction case map corresponding to the constant applied stress conditions listed in Tab. 3.3. The x-axis refers to stress τ_{cs} acting on the cross-slip system and y-axis is the resolved stress τ_p acting on the primary slip plane. The 3 color codes are explained in the text. The results correspond to: (a) Set 1. (b) Set 2. (c) Set 3. (d) Set 4.

The strain evolutions corresponding to $L_{cs} = L_p = 150 \text{ nm}$ cases are shown in Fig. 3.11. Fig. 3.11a presents the time evolution of the total strain rate for $\tau_p = 120 \text{ MPa}$, for different τ_{cs} values ranging from 100 MPa to 180 MPa (Fig. 3.11a, curves B, C, D). These results are compared with the strain rate evolution of coplanar source case, using $L_p = 300 \text{ nm}$ (Fig. 3.11a, curve A). The cross-slipping time and the post-interaction strain rate strongly depend on the τ_{cs} level.

In Fig. 3.11b cases ($\tau_p = 180$ MPa), no dislocation source blocking (strain rate = 0) is observed (compared to Fig. 3.11a, curve A, for example). In addition, node C reaches node A for a significantly smaller τ_{cs} level, as compared to $\tau_p = 120$ MPa cases in Fig. 3.11a. If $\tau_{cs} < 160$ MPa (Fig. 3.11b curve B), segment BC directly cuts through the obstacle, generating a sharp strain rate jump at t = 0.12 ns. The second peak appears as the source is entirely transferred into the primary slip plane. In the $L_p = 300$ nm case (Fig. 3.11b curve A), the dislocation velocity is faster due to the lack of the competition between segments AC and BC. Similarly, in $\tau_{cs} > \tau_p$ case (Fig. 3.11b curve D), loop by-passing mechanism occurs with a slower strain evolution. The presence of the cross-slipped segment AC (for the case of $L_{cs} > 1/3L$) systematically helps the primary segment BC to get past the obstacle, including for τ_p and τ_{cs} levels below the critical obstacle strength τ_c (from Fig. 3.6: $\tau_c \sim 150$ MPa). This effect reduces with the decrease of the cross-slip segment length L_{cs} .

In order to evaluate the separate contribution of cross-slip on the dislocation-loop interaction strength, we finally replaced the $[1\overline{1}1]$ loop with a hard, impenetrable platelet (or facet). The facet position, size and orientation are exactly the same as those of the $[1\overline{1}1]$ loop. This part is detailed in Section 4.

3.2 Interaction with [111] loop

3.2.1 Interaction mechanism and obstacle strength: planar dislocation source

The screw dislocation without pinning points and periodic boundary condition case is first examined, using fixed strain rate conditions as in section 3.1.1. In this case, the dislocation loop is absorbed in the form of a helical turn (Terentyev et al., 2010) which then closes itself and leaves a [111] loop behind, as the screw dislocation breaks away. This mechanism is associated with a critical interaction stress $\tau_c = 0.72 \mu b/(L-D)$ in agreement with (Terentyev et al., 2010) (see Fig. 3.4).

The coplanar finite-length (pinned) dislocation source case is examined next (see Fig. 3.12). A helical turn is formed during the first stages of the interaction (Fig. 3.12b), then after a significant bow-out of the dislocation, the helical turn reconnects and reemits the initial loop in a process similar to Hirsch's mechanism (Smallman and Harris, 1977) (Fig. 3.12e). This configuration induces higher obstacle strength as compared to the [111] loop case, owing to the larger line tension build-up. The corresponding critical interaction stress $\tau_c = 240$ MPa could be obtained from the Eq. (3.8) taking $\alpha_{eff} = 0.72$ and $\alpha_{LT} = 0.25$. It is interesting to note that the helical turns move together with the bowed-out dislocation (Figs. 3.12c and 3.12d). As a result, the obstacle strength depends on the initial position L_2 (see Fig. 3.2). If $L_2 = L/2$ for example, the obstacle strength $\tau_c \approx (\alpha_{eff} + 1/\alpha_{LT})\mu b/(L - D)$ for $\alpha_{LT} = 0.48$ instead of 0.25. This means the [111] loop is released before the dislocation bow-out adopts a semi-circular configuration. Only $L_p = L_{cs} = 150$ nm case is presented hereafter, for simplicity. Different applied stress conditions (τ_p , τ_{cs}) are examined in the next section, for the composite source cases.



FIGURE 3.11: Total strain rate evolutions versus time associated with simulation setup 3 ($L_{cs} = L_p = 150 \text{ nm}$), for different loading combinations (τ_p , τ_{cs}). (a) $\tau_p = 120 \text{ MPa}$ and τ_{cs} varies from 100 to 180 MPa. (b) $\tau_p = 180 \text{ MPa}$ and τ_{cs} varies from 100 to 200 MPa. The different curves A, B, C, D are further described in the main text.



FIGURE 3.12: Interaction between a coplanar pinned dislocation source and a [111] loop. The (screw-type) dislocation source glides in the X direction ($[\bar{1}\bar{1}2]$ direction). A helical turn is formed in frame (b), which subsequently propagates towards point B, while AB segments glides and bows-out. The helical turn is released in frame (e). The interaction results in the net displacement of the initial loop, which is reformed near the pinning point B. the source length L = 300 nm.



FIGURE 3.13: Interaction between a composite dislocation source and a [111] loop. The source length $L_{cs} = 150 \text{ nm}$ for $\tau_p = 190 \text{ MPa}, \tau_{cs} = 160 \text{ MPa}$. The mobile screw dislocation segment BC glides in the X direction ([112] direction).

3.2.2 Interaction mechanism and effective obstacle strength: composite dislocation source

The results associated with $L_{cs} = 150 \text{ nm}$ case are presented in Fig. 3.14. In Fig. 3.14a, the critical stress range is comprised between 130 MPa and 280 MPa, in consistence with the strength of the helical turn mechanism. A fourth interaction mechanism is introduced in Fig. 3.14a (S=3, black color area), where the dislocation bow-out keeps gliding without the helical turn closure. In this case, one segment of the helical jog with the slip system $(1\overline{10})[111]$ is simply dragged away, since the loop and the incoming line share the same Burgers vector as shown in Fig. 3.13. Similarly, interaction strength of the composite source is lower than that in the coplanar source case, under comparable loading conditions (see also Fig. 3.14b).

Lastly, a simulation case where the [111] loop is replaced by a [111] oriented hard facet is carried out as well. It is recalled that unlike the loop, the facet has no associated stress field; whereas interaction with a facet involves none of the dislocation recombination mechanisms associated with loop interaction. This comparison further confirms that, in presence of cross-slip, the effective loop/obstacle interaction strength weakly depends on the loop-induced elastic stress field or the particular dislocation-loop interaction mechanism. For more details, please refer to Section 4.



FIGURE 3.14: Composite source interaction ($L_{cs} = 150 \text{ nm}$) with a [111] loop. (a) The different interaction mechanisms are indicated by different color, depending on the considered applied stress (τ_p , τ_{cs}) combination. Mechanisms S = 0, 1, 2, 3 are explained in the main text. (b) Total strain rate evolutions versus time for $\tau_p = 160 \text{ MPa}$ and τ_{cs} varying from 130 to 220 MPa. The interaction mechanism, the cross-slipping time and the post-interaction total strain rate strongly depends on the τ_{cs} level.

3.3 General discussion

The interaction mechanisms reported in Sections 3.1.1 and 3.2.1 involve un-dissociated dislocations and strictly no cross-slip contribution. In these conditions, it can generally be assumed that these DD and MD evolutions are strain-rate independent and therefore, applicable to much slower strain rate conditions (Terentyev et al., 2010, 2008; Shi et al., 2015; Nogaret et al., 2007). The results reported in Sections 3.1.2 and 3.2.2 are obtained under constant applied stress conditions, however. In the composite-source case studies, it is important to note that the simulation time originates immediately after the glide plane change of one of the incoming, mobile dislocation arms. In usual straining conditions, this glide plane change would take place after a definite dwell time (associated with the cross-slip mechanism) which is not counted in the total reaction time reported in Figs. 3.11 and 3.14b. Sections 3.1.2 and 3.2.2 results thus focus on the strain-rate independent steps of the interaction, which may be applicable to much slower strain rate conditions as well.

For instance, disperse defects were implemented in massive, grain scale calculations, based on high strain rate MD calculation results (Terentyev et al., 2010, 2008). Grain-scale simulations were then carried out at strain rates up to 5 orders of magnitude slower. The resulting dislocation microstructures and corresponding stress-strain response are, none-theless, fully consistent with available experimental evidence (Gururaj et al., 2015a,b; Li and Robertson, 2018). This situation can be rationalized by noting that most of the simulation time (or the actual, experimental time) is then spent waiting between the different cross-slip events. It is also important to note that strain reported strain rates strongly depends on the mobile dislocation density, according to the simulated space sizes. The situation is significantly different in massive DD calculations, where the mobile dislocation density is limited by interaction with various obstacles, thus limiting the mobile dislocation densities (Arsenlis et al., 2012).

As a concluding remark, all the results presented in Section 3 were obtained using the specific, materials-dependent parameters of Section 2. It can be shown, however, that cross-slip mechanism affects dislocation/loop interactions in a wide range of BCC alloys (see for example: Robertson and Meslin (2011); Robertson et al. (2007); Farrell (2003)), corresponding to different sets of physical, material parameters (see Tab. 3.2). The reported cross-slip effect is in any case active and mainly depends on the sub-grain stress landscape, acting on the incoming (screw) dislocation arms (Gururaj et al., 2015a,b; Li and Robertson, 2018).

4 Effect of the absence of loop-induced stress field

In this section, we will study the separate contribution of the loop-induced stress field on such dislocation/loop interactions. These loops have thus been replaced by hard impenetrable platelets (or facets) as shown in Fig. 3.15, without any associated elastic stress field. At first for the periodic boundary condition case, the interaction between a screw dislocation and a facet corresponds to the Orowan mechanism: the two long dislocation arms reconnect past the hard facet and a loop debris is left behind. The corresponding



FIGURE 3.15: Simulation volume configuration for facet cases (the coordinate system is identical to loop cases as illustrated in Fig. 3.1b).

interaction strength is consistent with Orowan's expression (Bacon et al., 1973) (Fig. 3.4 for example of $[1\overline{1}1]$ facet case).

For the rest of this chapter, we shall focus on the motion of the composite dislocation source rather than the effective obstacle strength, which will then be treated in the next chapter (please refer to Fig. 4.5c for more details).



FIGURE 3.16: Total strain rate evolutions versus simulation time associated with simulation setup 3 ($L_{cs} = L_p = 150 \text{ nm}$), for different loading combinations (τ_p , τ_{cs}), i.e. $\tau_p = 120 \text{ MPa}$ and τ_{cs} varies from 100 to 180 MPa. The different curves A, B, C, D are further described in the main text.

4.1 Interaction with $[1\overline{1}1]$ facet

This section focuses on dislocation interaction with $[1\bar{1}1]$ oriented facet. The composite dislocation source case is systematically investigated using different setups shown in Tab. 3.3. The strain rate evolutions of Set 3 are shown in Fig. 3.16 for $\tau_p = 120$ MPa and different τ_{cs} values ranging from 100 to 180 MPa (curves B, C, D). These results are compared with the coplanar dislocation source case using $L_p = 300$ nm (curve A). The strain rate peak visible in curve B indicates the time where the initial source is entirely transferred into the primary slip plane and then, blocked by the interacting facet (as in curve A case); whereas the strain rate peaks in curves C and D indicate the time where the initial source is entirely transferred into the cross-slip plane and thereby, by-passes the facet. The critical interaction stress is clearly affected by the presence of a cross-slipped segment. Moreover, the strain rate peak time is shifted by about 0.04 ns when compared to the loop case, as compared to Fig. 3.11a. This means that the reaction completion time is up to 15% shorter than the actual loop case, depending on the loading conditions.

The total strain and corresponding total strain rate evolutions are shown in Fig. 3.17 for $L_{cs} = L_p = 150$ nm and loading stresses $\tau_{cs} = \tau_p = 120$ MPa. These conditions are typically found in a Fe specimen loaded in uniaxial tension, after irradiation up to $\sim 10^{-3}$ dpa at 300 K (Victoria et al., 2000). In the early stage of the interaction, segment BC glide is aided by the loop-induced stress field, up to marker (1). Node C quickly attains the junction segment formed by segment BC interaction with the loop, in (2). At this point, the local stress field and the junction hinder the continuous movement of node C, which retards the transfer of segment AC towards the cross-slip plane, in (3) and (4). In the facet case for comparison, segment AC displacement is rather continuous, until it is entirely transferred into the cross-slip plane, after ~ 1.2 ns. The reaction time is nearly the same in the loop case (several ps shift), with a relative total strain error of about 3%. Interaction with $[1\bar{1}1]$ loop or facet is thus controlled by the cross-slip mechanism.

4.2 Interaction with [111] facet

The different interaction mechanisms associated with the $L_p = 150$ nm case are presented in Fig. 3.18, for the applied stress range is comprised between 130 and 280 MPa, in agreement with the prior interaction strength result (since the source can overcome the obstacle in the primary slip system if $\tau_p > 210$ MPa). Compared to the actual loop case presented in Fig. 3.14a, only three different interaction mechanism are here observed (the helical turn formation mechanism is therefore missing). The interaction strength of the composite source is again lower than that in the coplanar source case, under comparable loading conditions.

Lastly, interactions with [111] loop and [111] oriented hard facet are compared side to side, in Fig. 3.19. The interaction curves are much more continuous (flatter) than in Fig. 3.17 due to the small effective contacting obstacle size, minimizing the number of node insertion operations. It is recalled that unlike in the loop interaction case, the facet case does not generate any stress field and excludes the helical jog formation. The



FIGURE 3.17: Total strain (upper frame), total strain rate (lower frame) evolutions and corresponding dislocation configurations. This case corresponds to $L_{cs} = L_p = 150$ nm and loading condition $\tau_{cs} = \tau_p = 120$ MPa. The loop and facet cases are denoted by solid and dashed lines, respectively. In the loop case, the junction is formed in (1), as the mobile dislocation segment is attracted by the loop; in (2): the common node C approaches the loop; in (3): the dislocation segment unpins from the loop; in (4): the dislocation is entirely transferred into the cross-slip plane. For the facet case, in I: the common node C moves close to the facet; in II: the dislocation segment by-passes the facet; in III: the dislocation is entirely transferred into the cross-slip plane. The small fluctuations taking place between II and III (or (3) and (4)) are due to the discrete description of the dislocation segments (node insertion or removal).



FIGURE 3.18: Composite source interaction ($L_p = 150$ nm) with a [111] facet. The different interaction mechanisms are indicated by different color, depending on the considered applied stress (τ_p , τ_{cs}) combination. S = 0: the source is blocked by the obstacle; S = 1: the dislocation goes through the facet in the primary slip plane; S = 2: the source overcomes the facet while gliding in the cross-slip plane. The present results apply to room temperature straining conditions.

reaction completion time presents a 0.1 ns time shift, between dislocation/loop and dislocation/facet cases. The corresponding relative total strain difference is less than 12%, between the two aforesaid cases.

4.3 General discussion

The loop-induced stress field generally contributes to the dislocation/loop interactions. This contribution can be summarized as follows:

- 1. In the presence of cross-slip (composite source), the dislocation/obstacle interaction time is up to 15% longer for a given loop case, with respect to the corresponding facet case. This effect is analogue to adding an extra viscosity, during the whole interaction time. The total reaction time of the [111] facet case with B = 0.14 MPa \cdot ns is indeed identical to that of the [111] oriented loop case;
- 2. The total strain shift is up to 12% smaller for a given loop case with respect to the corresponding dislocation/facet case. This effect is mainly ascribed to the actual loop displacement, during the interaction time. In the [111] oriented loop case for example, this corresponds to the formation and propagation of a helical turn. The loop-induced stress field has therefore little effect on stress-strain response associated with the dislocation/loop interaction.



FIGURE 3.19: Total strain (upper frame), total strain rate (lower frame) time evolutions and corresponding dislocation configurations. The represented case corresponds to $L_p =$ 150 nm with loading condition $\tau_{cs} = \tau_p = 120$ MPa. The loop and facet cases are denoted by solid and dashed lines, respectively. In the loop case, the helical jog is formed in (1), where the mobile dislocation segment is attracted by the loop; in (2): the former helical jog is closed itself and then the dislocation is entirely transferred into the cross-slip plane. In the facet case, in I: the dislocation segment by-passes the facet; in II: the dislocation is entirely transferred into the cross-slip plane.

In the composite dislocation source configuration, dislocation/loop interaction mainly depends on node C displacements, which is not significantly affected by the loop-induced stress field, regardless of the interacting loop orientation. Cross-slip is then a major strain rate limiting mechanism, in the investigated case studies.

The critical interaction stress is much weaker in presence of cross-slip, as reported in (Shin et al., 2003; Kelly and Nicholson, 1971). This effect could then explain grain scale plasticity mechanisms (Gururaj et al., 2015b) and in certain conditions, the corresponding stress-strain response of post-irradiated materials (Li and Robertson, 2018). Dislocation mobility in presence of defect dispersion and cross-slip is accurately described using the proposed, simplified dislocation/facet description. This approach can significantly improve the computational efficiency in massive (grain scale) DD simulations (Gururaj et al., 2015a).

5 Conclusions

Interactions between screw-type dislocation sources with $[1\bar{1}1]$ and [111] loops and facets are investigated using 3D nodal dislocation dynamics simulations. The comparative interaction strength levels associated with $[1\bar{1}1]$ and [111] obstacles are evaluated using coplanar source cases first, where all the initial source segments glide in the same primary slip plane. Coplanar sources are used: I) infinitely long dislocation segments, due to the periodic boundary conditions, II) in the form of a finite-length, pinned dislocation segments. Case-I is adopted as a benchmarking case, for validating our DD simulation model and setup by comparison with well-established MD simulations results. It is found that interaction strength is significantly larger in finite-length source case (case-II) than in periodic boundary conditions case (case-I). Pinned source nodes induce a local dislocation curvature and associated extra line tension contribution, adding up to the total effective interaction strength.

The case of composite dislocation sources is further investigated. This configuration includes two distinct (L_p, L_{cs}) long segments, gliding in the primary and cross-slip planes, respectively. The effect of various loading conditions (τ_p, τ_{cs}) on the effective interaction strength is examined, in terms of interaction mechanisms and time evolution of the strain rate. It is shown that the presence of a cross-slipped segment L_{cs} could systematically reduce the resolved shear stress needed to unpin the screw dislocation if $L_{cs} > 1/3L$, regardless of the particular loop-induced interaction mechanism and loop-induced stress field.

Finally, the SIA loops have been replaced by impenetrable facets to investigate the stress field effect on the composite source activation. It is found that the loop-induced stress field has little effect on the composite source operation.

In conclusion, the present results indicate that cross-slip is possibly the dominant strain rate limiting mechanism, in presence of disperse loop populations. The corresponding local interaction mechanisms are consistent with grain scale DD simulations results, in terms of post-irradiation plastic strain spreading.

Chapter 4

Effective dislocation mobility in post-irradiated ferritic grains

This chapter is reproduced from:

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Yang Li, Christian Robertson, Xianfeng Ma, Biao Wang (2019). Dislocation spreading and ductile to brittle transition in post-irradiated ferritic grains: Investigation of grain size and grain orientation effect by means of 3D dislocation dynamics simulations. Journal of Materials Research, 34, 1584.

In this chapter, post-irradiation plastic strain spreading at the grain scale is carried out by means of segment-based dislocation dynamics (DD) simulations, adopting the loopfacet surrogate technique presented in Chapter 3. The defect-induced evolutions of the effective screw dislocation mobility are evaluated by means of statistical comparisons, yielding a quantitative Defect-Induced Apparent Straining Temperature shift (or Δ DIAT) level. The influence of various factors including the straining temperature, the grain size and grain orientation on the Δ DIAT magnitude is examined in detail. The Δ DIAT level associated with a given defect dispersion is then compared to the measured ductile to brittle transition temperature shift (Δ DBTT). The results are further analyzed in terms of dislocation-based plasticity mechanisms and their possible relations with the dosedependent changes of the ductile to brittle transition temperature.

1 Introduction

Ferritic steels are widely used as reactor pressure vessel materials (RPV), thereby submitted to dose-dependent evolutions including: embrittlement, hardening, ductility loss, swelling, etc. (Bloom, 1998; Matijasevic et al., 2008, 2009; Baluc et al., 2007). These materials have a well-defined ductile-to-brittle transition (DBT), which strongly depends on irradiation temperature and dose (Hishinuma et al., 1998; Nikolaev et al., 2002; Shiba and Hishinuma, 2000). In absence of radiation-induced defects, the temperature-dependent fracture response is ascribed to a given screw dislocation mobility level (Rice, 1992; Cleveringa et al., 2000; Tanaka et al., 2008). At fixed testing temperature T_0 however, the fracture toughness level K_0 is generally higher than its post-irradiated counterpart, K_1 (Matijasevic et al., 2008; Kuleshova et al., 2002). Interestingly, the usual experimental trend curves indicate that this $K_0 \rightarrow K_1$ evolution can be replicated in a non-irradiated specimens, by depressing the test temperature $T_0 \rightarrow T_1$ (where $T_1 < T_0$). This perception implies that the fracture toughness gap $K_0 \rightarrow K_1$ (at T_0) is possibly caused by a defectinduced shift of the effective dislocation mobility.

The exposure of metallic materials to neutron irradiation flux results in the progressive accumulation of radiation-induced defect clusters, mostly in the form of dislocation loops. These defect clusters can then strongly interact with dislocation-mediated plasticity mechanisms, according to transmission electron microscopy (TEM) observations (Gaganidze and Aktaa, 2013; Robach et al., 2003), molecular dynamics (MD) (Bacon and Osetsky, 2005; Terentyev et al., 2008) and dislocation dynamics (DD) (Greer et al., 2008; Ghoniem et al., 2001; De la Rubia et al., 2000) simulations. Several grain-scale plasticity mechanisms in post-irradiated bcc metals have been conducted in the past few years (Yefimov et al., 2004; Chaussidon et al., 2008; Arsenlis et al., 2012; Gururaj et al., 2015b). A statistical description of dislocation mobility in presence of dispersed defects and how it possibly relates to the ductile to brittle transition temperature are missing, however. The purpose of this work is thus to explore the analog effect of straining-temperature and dispersed defect populations on dislocation mobility, using three-dimensional DD simulations.

Current surveillance practices include the DBT temperature assessment of the RPV steel. Such evaluation involves the destructive testing of a fixed number of macroscopic specimens, inserted in surveillance capsules located near the RPV inner wall, prior to the initial reactor start-up. The surveillance specimens are taken out-of-pile at a selected periodicity (a few years, typically) and then handled, tested and disposed of in hot cell facilities (Yoo et al., 2015; Ballesteros et al., 2014; Alshits and Indenbom, 1986). Though reliable, this conventional approach is time-consuming, extremely costly and lacks flexibility.

The ultimate goal is therefore to develop and apply supporting evaluation methods, preferably based on numerical simulation and non-destructive observation techniques like EBSD analysis (Diaz-Fuentes et al., 2003), SANS measurements (Meslin et al., 2010; Heintze et al., 2010) or X-ray submicron diffraction methods (Budiman et al., 2006; Khoo et al., 2016; Tippabhotla et al., 2017), for example. Such approach could then help opti-

mizing the existing surveillance programs, while providing valuable complementary information regarding the material degradation causes. This work is regarded as an essential step towards developing a fully predictive model, applicable at the scale of representative (macroscopic) grain aggregates and then, macroscopic specimens (Viehrig et al., 2002).

The present chapter contains four core sections. Section 2 presents the adopted investigation methodology, including : the thermally-activated dislocation mobility rules (Section 2.1), the different simulation setups (Section 2.2), the defect-induced apparent straining temperature shift (Δ DIAT) concept (Section 2.3). Section 3 presents the DD simulation results of 1- μ m³ grains with different defect dispersions, including : the stress-strain response and dislocation density spreading (Section 3.1), the effective resolved shear stress and dislocation velocity evolutions (Section 3.2), the associated Δ DIAT trends (Section 3.3) and its physical interpretation (Section 3.4). Section 4 shows the role of other factors in the DIAT scenarios, including: the straining temperature (Section 4.1), the grain size (Section 4.2) and grain orientation (Section 4.3) effects. Comparisons between Δ DIAT and Δ DBTT are lastly shown in Section 5, together with discussions on their correlation.

All these studies are adapted to Fe-2.25%Cr grains taken as a model ferritic system, for which all the required data is available in the open literature (see also Section 2), as far as dislocation mobility is concerned.

2 Model and method descriptions

2.1 Dislocation mobility rules

The present 3D dislocation dynamics simulations were performed using TRIDIS code, where the dislocation lines are described through series of discrete linked sections, in the form of orthogonal edge and screw segments (Verdier et al., 1998).

These segments glide in discrete body center cubic lattice, where the lattice spacing parameter corresponds to 10 times the Burgers vector magnitude *b*. The dislocation segment lengths correspond to discrete multiples of the lattice spacing, capturing the complexity of the dislocation network caused by all the implemented obstacles. The displacement of a mobile segment during a given time step is calculated according to its stress-dependent velocity. It is usually assumed that screw dislocation velocity in bcc metals is controlled by thermally activated, kink pair nucleation. The corresponding stress-velocity rule used in our DD simulations has been described in (Gilbert et al., 2011; Tang and Marian, 2014), where the screw segment velocity is given by:

$$v_{screw} = hJX' \tag{4.1}$$

where *h* is the Peierls valley width, *J* is the kink pair nucleation rate per unit dislocation length and X' is the kink pair propagation distance before annihilation with an opposite propagating kink pair, along a screw dislocation of finite length. In practice, this length is

taken as:

$$X' = \frac{X_{\infty}L}{X_{\infty} + L} \tag{4.2}$$

 X_{∞} is the average (and finite) distance swept by a kink pair before annihilation with another kink pair along an infinitely long screw dislocation; and *L* is the finite length of the dislocation segment considered. Distance X_{∞} can be expressed as:

$$X_{\infty} = 2\left(\frac{v_k}{J}\right)^{1/2} \tag{4.3}$$

where v_k is taken as equal to the (stress-dependent) edge dislocation velocity; while J is calculated as explained in references (Gururaj et al., 2015b; Gilbert et al., 2011), namely:

$$J(\tau^*, T) = \frac{8\pi (\tau^*)^2}{\mu B h} \exp\left(-\frac{\Delta G(\tau^*)}{k_B T}\right)$$
(4.4)

The pre-factor appearing in Eq. (4.4) can be interpreted as the kink-pair area generated per unit of time; *B* is the viscous drag coefficient, μ is the shear modulus, k_B the Boltzmann's constant, *T* is the test temperature, τ^* is the effective resolved shear stress acting on the dislocation segment considered and ΔG the kink-pair formation enthalpy (Gururaj et al., 2015b). The latter quantity is calculated using the following Kock's expression:

$$\Delta G(\tau^*) = \Delta H_0 \left[1 - \left(\frac{\tau^*}{\tau_0}\right)^p \right]^q \tag{4.5}$$

where ΔH_0 and τ_0 are the kink-pair formation energy and Peierls shear stress at 0 K. Quantities *p* and *q* characterize the shape of the thermal activation barrier, being either sharp or more gradual, with respect to τ^* variations (Tang and Marian, 2014).

Using fixed strain rate loading conditions means $\dot{\varepsilon} = \rho_{mobile}vb = constant$ and implies that $\Delta G(\tau^*) \approx Ck_BT$ (see Eq. (4.4)), where quantity *C* is a dimensionless, materialdependent scaling factor. This condition applies at least at low straining temperature, where $L \ll X_{\infty}$ (Tang and Marian, 2014). Inserting $\Delta G = Ck_BT$ in the left-hand part of Eq. (4.5) and solving for τ^* yields:

$$\tau^*(T) = \tau_0 \left[1 - \left(\frac{Ck_B T}{\Delta H_0} \right)^{1/q} \right]^{1/p}$$
(4.6)

Quantity $\tau^*(T)$ here scales with the material yield stress evolution with temperature. The bracketed term vanishes at $T = T_{athermal}$ and then:

$$T_{athermal} = \Delta H_0 / Ck_B \tag{4.7}$$

Inserting Eq. (4.7) in Eq. (4.5) taking p = 0.5 and q = 1 (based on atomistic calculations (Gilbert et al., 2013)) and differentiating with respect to *T* finally gives:

$$\frac{d\tau^*}{dT} = -\frac{2\tau_0}{T_{athermal}} \left(1 - \frac{T}{T_{athermal}}\right)$$
(4.8)

parameter	symbol	value
Kink pair formation enthalpy	ΔH_0	$4.86 \times 10^{-20} \text{ J}$
Mobility parameter	р	0.5
Mobility parameter	q	1.0
Peierls stress	Δau_0	358 MPa
Burgers vector	b	2.54 Å
Young's modulus	E	210 GPa
Poisson's ratio	ν	0.3
Drag coefficient	В	$34 \times 10^{-5} \text{Pa} \cdot \text{s}$
Time step	Δt	10^{-10} s

TABLE 4.1: Mechanical and microscopic parameters of bcc Fe-2.25%Cr matrix.

The left-hand term in Eq. (4.8) can be evaluated by means of temperature jump tests, performed¹ at $T \ll T_{athermal}$. The scaling factor $C \approx 10$ in Fe-2.25%Cr and this value applies to both pre and post-irradiated conditions (Böhmert and Müller, 2002). This means Eqs. (4.1)-(4.5) holds true in presence (and in absence) of dispersed defects, at least for the defect size and number densities considered in this study. The materials parameters to be used hereinafter are listed in Tab. 4.1 below, yielding the gradual temperature-dependent stress-velocity evolutions as shown in Fig. 4.1.

In the present DD simulation framework, the effective resolved shear stress acting on a particular dislocation segment corresponds to : $\tau^* = \tau_{applied} + \tau_{internal}$, where $\tau_{internal}$ includes line tension and mutual dislocation-dislocation interaction contributions (Gilbert et al., 2013; Böhmert and Müller, 2002). The dose-dependent evolutions of τ^* are related to the defect-induced changes in the dislocation microstructures. Stress and temperaturedependent Eqs. (4.3)-(4.4) ensure the gradual stress-velocity response transition towards a phonon-drag regime, beyond room temperature (Gilbert et al., 2013; Tang and Marian, 2014; Po et al., 2016). These evolutions are qualitatively and quantitatively consistent with the tensile and fracture toughness properties of Fe and Fe-Cr alloys (Böhmert and Müller, 2002).

The thermally activated cross-slip mechanism accounting for the twinning-anti-twinning asymmetry is treated according to a specific procedure, whereby the glide plane of each screw dislocation segment is updated at every simulation time step. In practice, the cross-slip probability assigned to a given screw segment depends on the effective resolved shear stress acting in its primary slip system versus its counterpart acting in the cross-slip system, during the time step considered. All the details regarding the implemented cross-slip procedure and its effect on plastic strain spreading have been presented elsewhere (Chaussidon et al., 2008; Robertson and Gururaj, 2011; Chaussidon et al., 2010). Finally, the edge segment velocity is proportional to effective resolved shear stress, using the phonon drag coefficient *B* from Tab. 4.1.

^{1.} Where Eq. (4.5) applies without major modifications.



FIGURE 4.1: The temperature-dependent stress-velocity response implemented in the present DD simulations. The solid curves are representative of an isolated L = 500 nm long screw dislocation, for various straining temperatures within the ductile-to-brittle transition range. The dashed lines superimposed to this figure indicate two limit cases. Namely, the a-thermal "high-temperature" regime is characterized by the phonon-drag coefficient $B = 34 \times 10^{-5}$ Pa · s. The vertical dashed line at $\tau = \tau_0$ indicates the lattice friction stress level (or Peierls stress), at 0 K.

2.2 Simulation setup adapted to ferritic grains

2.2.1 Simulation volume

Fe-2.25%Cr steels usually adopt a "bainitic" microstructure, including 1-2 µm thick sub-laths (or platelets) (Kuleshova et al., 2002), with $D_g \times 10 \times 10$ µm³ typical lath dimensions (see Fig. 4.2a). This corresponds to relatively large DD simulation volumes and makes it computationally prohibitive to investigate the targeted dose domain (> 0.1 dpa at irradiation temperature 300 °C), using small computer systems. For example, simulating a $D_g \times 10 \times 10$ µm³ Fe-2.25%Cr lath irradiated to 0.1 dpa requires handling as many as 10⁵ defects. Lath-scale simulations were nevertheless carried out at low defect densities (representing < 10⁻⁴ dpa), for comparison and validation purposes (Chaussidon et al., 2008). We thereby checked that the shear band structures generated in D_g -µm³ cubic grains are exactly the same as in bainitic laths, in terms of shear band thickness, mobile and stored dislocation densities (see for example Fig. 10 in Chaussidon et al. (2010)). In this work, D_g -µm³ cubic DD simulation volumes are thus implemented and tested (Fig. 4.2b) as listed in Tab. 4.2.



FIGURE 4.2: Adopted DD simulation setup. (a) Schematic representation of typical ferritic-bainitic steel microstructure and simplified cubic grain setup. The individual laths are included within lath blocks, where the inter-lath disorientation is minimal. (b) DD simulation setup representative of a D_g -µm³ cubic grain including a population of dispersed defects. This case includes 500 defects, with defect diameter D = 50 nm. In Fe-2.5%Cr this represents a 1 dpa at $T_{irr} = 400$ °C (Kuleshova et al., 2002).

Direct TEM observations have shown that the strain-induced dislocations are mostly confined inside of the individual laths, up to significant macroscopic tensile strain levels, regardless of the internal coherency stresses coming from the other grains (Gururaj et al., 2015b,a; Robertson et al., 2007). Using impenetrable grain boundaries allows for a realistic description of intra-granular stress field and accompanying the formation of the sub-structure, during DD simulations of bainitic-ferritic grains (Robertson and Gururaj, 2011). Further evidence supporting these claims is presented in Jiang et al. (2019), where the grain shape effect on the plastic response has been investigated in detail. The use of small cubic grain is thus preferred, for the sake of minimizing the computational load.

2.2.2 Irradiation defect implementation and dislocation-defect collision treatment

Irradiation defect clusters in Fe-Cr alloys mainly develop in the form of interstitial loops, at high irradiation temperature (> 300 °C). Back at room temperature, these clusters are trapped by impurities and can be regarded as immobile obstacles, with respect to mobile dislocations. The defect dispersion characteristics depend on many different factors such as the irradiation temperature, material chemical composition and cumulated dose (Matijasevic et al., 2008; Kuleshova et al., 2002).

Our calculations do not assume any particular dose-density dependence, however. It is simply presumed that each implemented defect density correspond to only one, specific dose level. Loops orientations $\langle 100 \rangle$ and $1/2\langle 111 \rangle$ were both present in Fe-Cr alloys at $T_{irr} = 300 \,^{\circ}$ C (Xu et al., 2009). The proportion of $\langle 100 \rangle$ loops is higher in Fe-Cr alloys than in pure Fe, for a given irradiation temperature. The proportion of $\langle 100 \rangle$ over $\langle 111 \rangle$ loops also increases with T_{irr} so $\langle 100 \rangle$ orientation becomes dominant for T_{irr} in the 350-450 °C range (Kocik et al., 2002).

In this work, the radiation defects clusters are implemented in the form of soft internal obstacles called facets (planar, square-shaped surfaces as shown in Chapter 3). We firstly checked that for a given facet size, changing the facet orientation or taking a random combination of facet orientation has no effect on grain-scale plastic strain spreading. And hence, all the facet planes are orientated normal to the (100) direction, for simplicity. Each time a dislocation-facet collision is detected, the total effective shear stress applied on the dislocation line τ^* is compared with the critical facet strength τ_{defect} . Mobile dislocations cut through to the facets if $\tau^* > \tau_{defect}$. The selected τ_{defect} level is calibrated using a simple simulation procedure, where one dislocation line is interacting with 2 facet-loops (Robertson and Gururaj, 2011). In that case, the facet diameter and spacing is fixed (for example: D = 20 nm and loop spacing LS = 80 nm), while the facet strength

TABLE 4.2: The different DD simulations setup cases treated in this work.

Grain 1	Grain 2	Grain 3
$D_g = 1 \mu m$	$D_g = 2 \mu m$	$D_g = 2 \mu m$
z-axis = (100)	z-axis = (100)	$z\text{-axis} = (\bar{1}54)$

Dislocation-mediated plasticity mechanisms analyzed by dislocation dynamics simulations

 $\tau_{defect} = \infty$ (hard facet case). This particular configuration yields a critical shear stress $\tau_{Orowan} = 95$ MPa, in good agreement with the continuum theory (Bacon et al., 1973). MD calculations show that defect loop resistance to dislocation motion generally depends on the mobile dislocation character (Terentyev et al., 2009). For each implemented facet number density (spacing) and size, τ_{defect} is set to 2.26 times τ_{Orowan} for screw dislocations (Terentyev et al., 2010) and 0.7 times τ_{Orowan} for edge dislocations (Terentyev et al., 2008). The reader should note that such obstacle strength is kept constant throughout the simulation. As evidenced by MD simulations (Terentyev et al., 2010), SIA loops are generally released after the dislocation/loop reaction completion, even in formation of the helical turn.

The simple dislocation/defect treatment adopted here bears several practical advantages, including: i) it correctly deals with the dislocation/defect interaction mechanisms affecting the grain-scale plasticity mechanisms, even though the facets do not generate any stress fields, ii) it allows using a comparatively much larger simulation time step compared to that required for a detailed dislocation/defect interaction treatment (typically 10^{-10} s instead of 10^{-12} s) (Gururaj et al., 2015a). Importantly, we have shown that in presence of cross-slip, the implemented facet-loop treatment is able to capture the overall dislocation velocity and stress-strain response changes due to disperse defect interaction (Chapter 3). This assertion appears to hold true regardless of the actual interaction mechanism (Gururaj et al., 2015a), including the defect-induced elastic stress field effect (Shin et al., 2003).

2.2.3 Loading conditions and simulation cases

Uni-axial tension is applied along the (100) direction and the stress magnitude is feedback controlled in a bid to keep the constant plastic strain rate with $\dot{\epsilon} = 100 \,\mathrm{s}^{-1}$. Different irradiation conditions are simulated by inserting different defect number densities $(3 \times 10^{20} - 6 \times 10^{21} \mathrm{m}^{-3})$ and defect sizes $(5 - 50 \mathrm{nm})$ (Kuleshova et al., 2002; Rieth et al., 1998; Gupta et al., 2006; Meslin, 2007). Simulation with grain sizes of 1 µm (Grain 1) and 2 µm (Grain 2 and Grain 3) have been carried out. Grain 2 and Grain 3 have two different crystallographic orientations: in the first case (Grain 2), the grain z-axis is orientated along the (100) direction. In the second case (Grain 3), the grain z-axis is orientated along the $(\bar{1}54)$ direction. In all the cases, 1-12 initial dislocation sources (with length ~ 100 nm) are randomly positioned in the grain, which belong to the a/2 (101)[$\bar{1}\bar{1}1$] slip system (SS), associated with cross-slip systems a/2($1\bar{1}0$)[$\bar{1}\bar{1}1$] and a/2(011)[$\bar{1}\bar{1}1$]. The Schmid factors corresponding to the two selected crystallographic orientations are indicated in Tab. 4.3. All the further simulations presented in this chapter are carried out at 300 K, unless specified otherwise.

2.3 Screw dislocation velocity distribution and DIAT shift concept

The influence of defect dispersions on the statistical screw dislocations mobility distribution can be associated with a certain Defect Induced Apparent straining Temperature

Slip system label	First SS	Second SS	Third SS
Slip system	$(101)[\bar{1}\bar{1}1]$	$(1\overline{1}0)[\overline{1}\overline{1}1]$	$(011)[\overline{1}\overline{1}1]$
z-axis = (100) Grain 1, 2	0.41	0.41	0
z -axis = ($\overline{1}54$) Grain 3	0.378	0.472	0.095

TABLE 4.3: Schmid factors acting in the different slip systems submitted to a (100) tensile loading, for the different DD simulations cases tested in this work.

(or DIAT) shift. This concept derives from the well-known ductile to brittle transition temperature shift (or Δ DBTT) notion, utilized in the context of post-irradiation fracture toughness testing (see Section 1). The proposed calculation method takes advantage of the above described (screw) dislocation mobility model, adapted to controlled strain rate loading conditions. The DIAT shift associated with a given defect dispersion is calculated in three distinct steps, as follows:

Step 1. The average stress $\overline{\tau_0^*}$ and dislocation velocity $\overline{v_0}$ levels are calculated in defectfree conditions (subscript 0) and at straining temperature T = 300 K, accounting for all the screw dislocation segments generated during all the time steps, up to the completion of a reference plastic strain level. In the present simulation conditions, the screw dislocation segment length L (~ 100 nm) is usually much larger than X_{∞} (~ 10 nm, based on Eq. (4.3)). According to Eq. (4.2), the kink-pair propagation distance $X' \approx X_{\infty}$ provided $L \gg X_{\infty}$. The average dislocation velocity $\overline{v_0}$ corresponding to $\overline{\tau_0^*}$ can then be calculated using:

$$\overline{v_0} = \alpha h J_0 X_{\infty,0} \tag{4.9}$$

where α is a dimensionless parameter (comprised between 0.9 and 1.0). More explicitly, this means:

$$\overline{v_0} = \alpha h J_0 X_{\infty,0} \left(\overline{\tau_0^*}, T_0\right) = \beta \overline{\tau_0^*}^{3/2} \exp\left(-\frac{\Delta G_0 \left(\overline{\tau_0^*}\right)}{2k_B T_0}\right)$$
(4.10)

where $\beta = 16 \alpha \pi (b/\mu^2 B)^{1/2}$.

The reader should bear in mind that $\overline{v_0}$ can be calculated with reasonable accuracy using Eq. (4.10) thanks to the selected simulation conditions (fixed strain rate and T = 300 K), where the stress-velocity response is quasi-linear, especially for $\tau^* > 50$ MPa (see Fig. 4.1). We further checked that $\overline{v_0}$ calculated directly from simulations differ by no more than 5% with respect to using Eq. (4.10) with $\overline{\tau_0^*}$ at 300 K.

Step 2. The effective resolved shear stress τ_1^* and corresponding velocity v_1 are then extracted in presence of defect dispersions (subscript 1), at the same straining temperature (T = 300 K) as before. Each (τ_1^*, v_1) combination is evaluated for each screw segment, based on:

$$v_1 = \alpha h J_1 X_{\infty,1} \left(\tau_1^*, T_1 \right) = \beta \tau_1^{*3/2} \exp\left(-\frac{\Delta G_1 \left(\tau_1^* \right)}{2k_B T_1} \right)$$
(4.11)

Recombining the Eq. (4.10) and (4.11) then yields:

$$\frac{\overline{v_0}}{v_1} \left(\frac{\tau_1^*}{\overline{\tau_0^*}}\right)^{3/2} = \exp\left(\frac{\Delta G_1}{2k_B T_1} - \frac{\Delta G_0}{2k_B T_0}\right)$$
(4.12)

It is important to note that Eq. (4.12) applies to individual dislocation segments and for a specific time step². The deviation of each (τ_1^*, v_1) combination with respect to $(\overline{\tau_0^*}, \overline{v_0})$ is related to a definite apparent straining temperature T_1 , solving Eq. (4.12). The corresponding defect-induced apparent shift of the straining temperature is then simply $\Delta T = (T_0 - T_1)$. This operation is repeated for all the screw segments generated, up to exactly the same reference plastic strain level as used for calculating the reference velocity $\overline{v_0}$. It is also important to note that Eq. (4.12) imposes that $X'_1 = X_{\infty,1}$ and $X'_0 = X_{\infty,0}$ (see Eq. (4.3)). This condition ensures that the a-thermal contribution of dislocation/defect collision is discarded, in the evaluation of T_1 . Dislocation/defect collisions indeed cause a-thermal changes of v_1 by disturbing the dislocation length distribution (see Fig. 4.6). This effect is distinct from the "thermal-like" defect-induced $(\tau_0^*, v_0) \rightarrow (\tau_1^*, v_1)$ contribution (see Eq. (4.4) and Section 3.3).

Step 3. The Δ DIAT level associated with a given simulation setup corresponds to the most typical ΔT variation amidst the whole, strain-induced (screw) dislocation population generated throughout the simulated time. Statistically, the Δ DIAT level corresponding to a given defect dispersion is then:

$$\Delta \text{DIAT} = \sum_{\tau_{\min}^*}^{\tau_{\max}^*} \left[\sum_{L_{\min}}^{L_{\max}} \Delta T \left(L, \tau^* \right) p \left(L, \tau^* \right) \right]$$
(4.13)

where τ^* is the effective stress acting on a given screw segment; $\Delta T (L, \tau^*) = (T_0 - T_1)$ is apparent straining temperature shift and $p(L, \tau^*)$ its corresponding, normalized probability of occurrence. This statistical and comparative Δ DIAT method yields stable results (see Fig. 4.5b) including in presence of crack-like discontinuities, provided the compared situations (with and without dispersed defects) assume exactly the same grain size and orientation.

The present Δ DIAT concept does not imply that dislocation interaction with dispersed obstacles and thermally activated lattice friction are actually the same physical mechanisms. It implies that dislocation/defect interactions are however equivalent to a definite temperature reduction, in terms of statistical, thermally activated (screw) dislocation velocities. From the author's standpoint, this defect/temperature equivalency can greatly facilitate the prediction of dose-dependent DBT temperature shifts, based on observation results (see also Section 5).

To the best of the author's knowledge, there is currently no experimental technique enabling direct evaluation of dislocation population mobility, let alone their characteristic,

^{2.} The reader should note that (τ_1^*, v_1) is generally not equivalent to $(\overline{\tau_1^*}, \overline{v_1})$.



FIGURE 4.3: Typical defect-dependent evolutions according to DD simulations. (a) Stress-strain evolution. (b) Dislocation density evolution with cumulated plastic strain. The defect number density corresponding to the 500 defects case is $5 \times 10^{20} \text{m}^{-3}$.

dose-dependent evolutions. An atomic-scale model has been recently developed, explaining the brittle-ductile transition based on isolated dislocation/obstacle interaction cases (Swinburne and Dudarev, 2018). This model confirms that defect-induced dislocation mobility evolutions can help revealing/evaluating the brittle-ductile transition evolutions.

3 Results and discussions: reference grain configuration

The results are grain size and grain orientation dependent. The simulations presented in this section are all obtained from the set of Grain 1 shown in Tab. 4.2.

3.1 Plastic strain spreading and stress-strain response

The stress-strain response of un-irradiated (defect-free) and irradiated simulation volumes (500 defects with D = 50 nm) are first compared side to side, as shown in Fig. 4.3a. In defect-free conditions, an applied stress level ~ 330 MPa is achieved for $\varepsilon_p > 5 \times 10^{-4}$, regardless of the number of initial dislocation sources (Gururaj et al., 2015b; Robertson and Gururaj, 2011).

This tensile stress magnitude corresponds to a 330MPa × 0.41 = 135MPa shear stress level (see Tab. 4.3). Subtracting the line tension contribution $\alpha_{LT}\mu b/L$ (where $\alpha_{LT} \sim 0.8$ for screw dislocations, whereas μ , *b* values are taken from Tab. 4.1), taking L = 500 nm and neglecting the dislocation-dislocation stress contribution yields an effective shear stress of about (135MPa - 32MPa) ≈ 103 MPa, acting on the mobile dislocations.

It is important to note that all the dislocation segments move according to Eqs. (4.1)-(4.5). In practice however, dislocation mobility is strongly obstacle-dependent, especially beyond $\varepsilon_p > 10^{-4}$ (see Fig. 4.3a) due to grain boundary, dislocation-dislocation and dislocation-facet interactions. And hence, only a small fraction of the dislocation segments present at (any) time step *N* actually move by more than 5 times the lattice spacing (10*b*), at time step *N* + 1. All the segments travelling a larger distance count in the mobile dislocation population, noted ρ_{mobile} . Since $\dot{\varepsilon} = \rho_{mobile}vb$ with $\dot{\varepsilon} = 100s^{-1}$ and v(103 MPa)at 300 K ~ 18 – 22m/s (from Fig. 4.1 or Fig. 4.4b), Fig. 4.3a data is consistent with $\rho_{mobile} = 2$ to $4 \times 10^{10} \text{m}^{-2}$. This means $\rho_{mobile}/\rho_{total} \sim 1\%$ to 2% based on Fig. 4.3b, in agreement with dislocation theory (Caillard and Martin, 2003) and direct experimental evidence (Robertson et al., 2007).

The strain-induced dislocation structures consist of individual shear bands, whose number and thickness increase with the plastic strain level and decrease with the defect number density (dose) (Gururaj et al., 2015b,a). This means the adopted DD simulation framework is able to capture the well-known strain localization trends and corresponding dislocation mobility evolutions (see Section 3.4).

In Fig. 4.3b, the dislocation density in the defect-free grain increases linearly and achieves $5 \times 10^{13} \text{m}^{-2}$ at $\varepsilon_p = 10^{-3}$. The dislocation accumulation rate is significantly larger in presence of defect dispersions (10^{14}m^{-2} at $\varepsilon_p = 10^{-3}$). This effect is associated with a significant increase of the applied stress level (see Fig. 4.3a), as reported in (Robertson et al., 2007; Maloy et al., 2001).

Mobile dislocation segments in strained grains are generally much longer than the disperse defect spacing. As a result, defect-contacting dislocation segments are connected to relatively long, defect free dislocation arms, positioned on either (or both) sides of a particular defect. Cross-slipping of the non-contacting (screw) arms generates out-of-plane segments and then super-jogs, at the time of dislocation unpinning (Gururaj et al., 2015b). This process repeats itself until coarser dislocation structures are formed, which can then act as new dislocation sources, enabling further plastic deformation. It can be shown that the strain-induced (coarsen-up) dislocation structures are consistent with the observed ones, despite the simplified dislocation-defect collision treatment adopted herein (Arsenlis et al., 2012; Gururaj et al., 2015b,a; Shi et al., 2015). Cross-slip thus appears to greatly facilitate dislocation unpinning from defects and contribute to the effective post-irradiation mobility of screw segments (see also Section 3.4).

3.2 Effective resolved shear stress and dislocation velocity: a statistical description

An output file is created for each DD simulation condition, representing a given radiation dose and irradiation temperature, depending on the defect size and number density (Matijasevic et al., 2008; Kuleshova et al., 2002). The effective resolved shear stress distributions of acting on screw dislocations are then calculated for 500 defects-50 nm, 2000 defects-20 nm, and 2000 defects-25 nm. The results presented in Fig. 4.4a combine each mobile screw segment and each simulated time step contribution. In the presence of irradiation defects, all the curves exhibit more or less the same mean value (below 100 MPa). By comparison, the mean stress level obtained in the absence of defects is approximately 122 MPa. The presence of defect dispersion thus tends to reduce the average



FIGURE 4.4: Various statistical distributions and their defect-dependent evolutions according to DD simulations. (a) Effective shear stress distribution acting on screw dislocations, (b) screw dislocation velocity distribution. The defect number density corresponding to the 500 and 2000 defects cases are $5 \times 10^{20} \text{m}^{-3}$ and $2 \times 10^{21} \text{m}^{-3}$, respectively. The effective shear stress data (Fig. 4.4a) is a direct output from the DD simulations and reflects the discrete nature of the dislocation/dislocation and dislocation/loop interactions. The dislocation velocity data (Fig. 4.4b) is indirect; i.e. calculated using non-linear and segment length-dependent Eqs. (4.1)-(4.5).

effective resolved shear stress acting on the dislocations. For an individual gliding dislocation under the deformation rate control, its shear stress must increase to overcome the obstacle. But here we investigate the motion of screw dislocation populations, where the situation is much more complicated due to the dislocation multiplication, propagation and interactions with obstacles. Therefore the decrease in the effective resolved shear stress is rationalized in terms of the generation of some short dislocations and the presence of the cross-slip as shown in Chapter 3. This particular point will be further discussed in Section 3.3.

The velocity distributions corresponding to the stress distributions in Fig. 4.4a are presented in Fig. 4.4b. The curve reaches the peak frequency at the velocity of 22 m/s in the absence of defects and exhibits a broader velocity distribution, in contrast with the irradiated grain cases. The broad dislocation velocity distribution obtained in the unirradiated (0 defect) case indicates that the dislocation lines can rearrange easily, within the simulated grain. In contrast, the sharper distribution observed in the 500 defects 50 nm case at 17 m/s is the signature of strain localization. Among all the results presented in Fig. 4.4, the 2000 defects and D = 25 nm case achieves the smallest average velocity and lowest effective resolved shear stress levels (i.e. the lowest average screw dislocation mobility).

3.3 DIAT shift and defect dispersions: a systematic investigation

Different defect number densities N are inserted in the Fe-Cr grains, using various defect sizes D ranging from 5 to 50 nm. The average effective shear stress evolutions are shown in Fig. 4.5a. For each defect size case, the average effective stress level decreases with increasing defect density, up to a saturation level. The effective stress evolution with increasing defect number density is weaker for smaller defect sizes: from 115 MPa (86 MPa) with $500 \times 10^{18} \text{m}^{-3}$ defects, down to 103 MPa (48 MPa) with $2000 \times 10^{18} \text{m}^{-3}$ defects, using D = 10 nm (and D = 25 nm), respectively. For fixed defect number density, the average effective stress augments with decreasing the defect size. More precisely, the lower stress level both depends on the defect size and number density, that is: 48 MPa for $2000 \times 10^{18} \text{m}^{-3}$ defects with D = 25 nm; as compared to 79 MPa for $5000 \times 10^{18} \text{m}^{-3}$ defects with D = 10 nm. Moreover, the $6000 \times 10^{18} \text{m}^{-3}$ -50 nm case, where the saturation stress is about 90 MPa can be compared to the $1000 \times 10^{18} \text{m}^{-3}$ -50 nm case, where the saturation stress merely reaches 38 MPa. These examples show that increasing the defect density and size have a qualitatively similar effect on screw dislocation velocity, though increasing the defect size is clearly more influential, according to the present results.

The defect-dependent evolutions of the effective screw dislocation mobility are then examined using the Δ DIAT concept as presented in Section 2.3. First, we checked that the Δ DIAT level is entirely independent of the reference plastic strain level, provided $\varepsilon_p > 5 \times 10^{-4}$ (see Fig. 4.5b and caption). The effect of the obstacle strength on the DIAT shift is presented in Fig. 4.5c. It is seen that the Δ DIAT sharply increases at small τ_{defect} , and attains a stable value around 80 K for $\tau_{defect} > 100$ MPa. This indicates that the obstacles strength has no effect on the DIAT shift as soon as the cross-slip mechanism is strongly activated.

The Δ DIAT values calculated based on Eqs. (4.12)-(4.13) are presented in Fig. 4.5d and show an opposite trend, with respect to Fig. 4.5a: a smaller effective stress level yields a lower apparent straining temperature and therefore, a larger DIAT shift. In the D = 50 nm case for instance, Δ DIAT steadily augments from 78 K for 300×10^{18} m⁻³ defects towards 98 K for 1000×10^{18} m⁻³ defects. The Δ DIAT shift evolutions are comparatively much smaller in the D = 5 nm case however, merely reaching 35 K for 6000×10^{18} m⁻³ defects. The Δ DIAT saturation levels are: 59 K, 81 K and 94 K for D = 10, 15 and 25 nm defect sizes, respectively. The DIAT shift thus achieves saturation for a critical defect number density, depending on the selected defect size.

The above-described Δ DIAT trends directly relate to the evolutions of state variables $L, v, \tau^*, T, \rho_{mobile}$ as schematically depicted in Fig. 4.6. Dislocation/defect collisions generate multiple dislocation sources (pinning points), fostering dislocation multiplication and accumulation (see Fig. 4.3b). This situation is associated with increasing mobile (and immobile) dislocation densities: $\rho_{m1} > \rho_{m0}$ based on microstructure evolution analysis. Taking fixed strain rate loading conditions implies that $\dot{\varepsilon} = \rho_m v b$ and therefore, $v_1 < v_0$ and $\tau_1^* < \tau_0^*$, in agreement with Fig. 4.4. This defect-induced $v_0 \rightarrow v_1$ evolution can be replicated in defect-free conditions, by changing the straining temperature $T_1 < T_0$ (see Section 2.3). In other words, the whole Δ DIAT concept implies that both defect interac-



FIGURE 4.5: Various defect-dependent evolutions according to DD simulation results. (a) Average effective resolved shear stress acting on the screw dislocation segments. (b) Effect of the reference plastic strain level on Δ DIAT magnitude. Stable results are achieved for plastic strain level $\varepsilon_p \sim 5 \times 10^{-4}$ corresponding to the onset of stable shear band formation, within the strained grains. (c) Effect of the obstacle strength τ_{defect} on Δ DIAT magnitude at $\varepsilon_p = \times 10^{-3}$ in the 500defects-50nm simulation case study. (d) Average DIAT shift evolution versus the defect number density *N* for various defect sizes *D*. Solid symbols : DD calculation results, dashed curves : semi-analytical adjustment using Eq. (4.14).

tion and straining temperature impact the dislocation mobility, even though dislocation interaction with defects is physically distinct from thermally-activated lattice friction.

The Δ DIAT levels obtained herein closely reflect the DBTT shift trends observed in fine-grained (~ 1 µm) ferritic materials, for corresponding defect dispersion evolutions. In irradiated Fe-2.25%Cr including $N = 4 \times 10^{21}$ defects/m³ with D = 5 nm for example, Δ DBTT = 20 K (Kuleshova et al. (2002): base metal VVER-1000 steel case). By comparison, Fig. 4.5d data indicates Δ DIAT = 20-22 K using exactly the same, experimentally observed defect dispersion characteristics. The present simulation results also apply to several fine-grained ferritic steels, with different chromium concentrations (other than 2.25%).



FIGURE 4.6: State variables v, τ^* , T and their qualitative defect-dependent evolutions, for a given $X' = X_{\infty}$ (see Eq. (4.3)).

In irradiated Fe-9%Cr including $N = 2 \times 10^{21}$ defects/m³ with D = 15 nm for example, Δ DIAT = 53 K is obtained, as compared to Δ DBTT = 48 K (Matijasevic et al., 2008). More generally, the Δ DIAT magnitude saturates for nearly the same material-dependent N and D figures as those associated with Δ DBTT saturation (Baluc et al., 2007; Rieth et al., 1998). The actual, dose-dependent fracture toughness shifts are then strongly correlated with the defect-induced evolutions of (screw) dislocation mobility, thus supporting of the main argument of this study.

More details regarding the Δ DIAT and Δ DBTT comparisons are presented in Section 5. The pronounced dependence of Δ DIAT on *N* and *D* parameters is discussed in the next section using an explicit, semi-analytical approach.

3.4 DIAT shift evolutions: a semi-analytical description and its physical interpretation

In principle, it is possible to develop a close-form expression describing the dosedependent Δ DIAT evolutions, based on the present DD results and Eqs. (4.12)-(4.13). In any case, this would include terms depending on the screw dislocation velocity distributions, which are generally not directly accessible to experimental evaluation. For this reason, a semi-analytical approach is preferred (see Fig. 4.5d: fitting curves), where:

$$\Delta \text{DIAT} = \Delta T_{\text{max}} \left(1 - \exp\left(-\frac{D}{\lambda}\right) \right) \left(1 - \exp\left(-d^2 D N\right) \right)$$
(4.14)
All the DIAT evolutions obtained herein can be satisfactorily described based on defect size D (in nm) and defect number density N (in m⁻³), using only 3 scaling parameters, namely: $\Delta T_{\text{max}} = 110$ K is a reference temperature shift; whereas $\lambda = 14$ nm and d = 219 nm are two characteristic distances. These 3 parameters apply to the whole investigated defect size range and can be interpreted as follows.

In metallic materials, the irradiation defect number density usually saturates beyond a certain dose, depending on the irradiation temperature. Quantity ΔT_{max} represents a reference DIAT shift level achieved: i) in absence of cross-slip, ii) assuming hard (nonshareable) disperse defects, iii) using N and D values representative of saturation irradiation conditions. The corresponding stress level $\tau_{Orowan,\text{max}}$ can be evaluated using Scattergood and Bacon expression (Bacon et al., 1973), with $D = 16 \text{ nm}, N = 2 \times 10^{22} \text{m}^{-3}$ and $L = 1/\sqrt{ND}$ (from Matijasevic et al. (2008)). Putting $\tau_1^* = \tau_{Orowan,\text{max}}$ and $v_1(\tau_1^*)$ (according to Eq. (4.11)) in Eq. (4.12) and then solving for T_1 yields: $(T_1 - T_0) = \Delta T_{\text{max}} \sim 110 \text{ K}$.

Cross-slip is the most efficient mechanism for generating the shear band structures as shown in Fig. 4.8 (as shown in details in Gururaj et al. (2015b)). These structures in turn generate an internal stress field, fostering local cross-slip activation (Gururaj et al., 2015a). In the rest of this section, it will be shown that the dose-dependent terms in Eq. (4.14) and corresponding Δ DIAT trends in Fig. 4.5d can be explained using a simple shear band model. The shear band induced stress (projected in the cross-slip system) can be described using a simple decay function (see also Fig. 4.8e):

$$\tau_{int}(y) \approx \left| \tau_{app} \exp\left(-k_{\max} \frac{|y|}{l}\right) \right|$$
(4.15)

where τ_{app} is the applied shear stress level, y is the distance normal to the shear band plane and $l \sim D_g/2$ (half) the grain diameter; quantity k_{max} is a dimensionless stress amplification factor, depending on the dislocation sub-structure type, i.e. $k_{max} = 1.75$ for dislocation tangles and $k_{max} = 5$ for dislocation pile-ups (Gururaj et al., 2015a).

Changing the grain size affects the dislocation sub-structure size l and corresponding internal stress field τ_{int} in agreement with Eq. (4.15). The corresponding Δ DIAT trends clearly indicate that terms $\exp(-D/\lambda)$ and $\exp(-d^2DN)$ from Eq. (4.14) actually scale with the internal stress field, depending on the sub-grain structures characteristic dimensions (tangle thickness and spacing). It can therefore be assumed that $\tau_{int}/\tau_{app} = \exp(-k_{\max}|y|/l) = \exp(-D/\lambda)$ where $k_{\max}|y|/l \approx D/\lambda$. Distance |y|/l satisfying this condition can be evaluated by determining λ independently, based on the integrated dislocation segment "flight distance" (see Fig. 4.7). Fig. 4.7 shows that $\lambda = 10.9$ nm which closely matches $\lambda = 11.4$ nm obtained by adjusting Fig. 4.5d data using Eq. (4.14). Quantity λ is mostly dose-independent in the tested simulation conditions, since it is much smaller than the typical defect spacing: $\lambda \ll 1/\sqrt{ND}$ (for $N = 6 \times 10^{21} \text{m}^{-3}$ and D = 15 nm). Overall, term $\exp(-D/\lambda) \approx \tau_{int}/\tau_{app}$ for a relatively long y/D_g range, given the typical D and λ values considered herein (see marker (1) in Fig. 4.8e).

Likewise, term $\exp(-d^2DN)$ in Eq. (4.14) can be interpreted as the τ_{int}/τ_{app} stress ratio solving Eq. (4.15) where $k_{\max}|y|/l \approx d^2DN$. Therefore, term $\exp(-d^2DN) \approx \tau_{int}/\tau_{app}$ wherever condition $k_{\max}|y|/l \approx d^2DN$ is satisfied. This corresponds to a relatively short



FIGURE 4.7: Integrated flight distance of screw segments in the presence of 500 defects with D = 50 nm. The recorded distances integrate the time (or strain) dependent velocity fluctuations of the screw segments moving in their initial glide plane up to complete arrest or up to a glide plane change, due to cross-slip. The mean flight distance corresponding to the presented distribution is ~ 10.9 nm.

y/l range (see (2) in Fig. 4.8e, where the mesh origin is positionned in the middle of the shear band) given the typical d^2DN values considered herein (see also Figs. 4.8a-4.8d and experimental comparisons (Rieth et al., 2013; Wei et al., 2002; Henning and Vehoff, 2005)). Parameters λ and d thus scale the internal stress field landscape and therefore, the dose-dependent trends predicted using Eq. (4.14). This analysis, based on Eq. (4.15) once more, highlights the crucial role of the cross-slip stress on post-irradiation plasticity (Xu et al., 2009; Kocik et al., 2002; Bacon et al., 1973).

4 Role of other factors

4.1 Straining temperature effect

In this section, we will discuss the straining temperature effect on the DIAT shift.

Defect-free grains (Grain 1) are simulated under three selected straining temperatures $T_0 = 250$ K, 300 K and 350 K (in DBT range). The corresponding stress-stain cures are presented in Fig. 4.9a, showing a pronounced applied stress amplitude decreases with increasing temperature. The corresponding dislocation density evolutions are shown in Fig. 4.9b: the total dislocation density linearly augments with the accumulation of plastic strain. The dislocation accumulation rate increases with straining temperature. For ins-



FIGURE 4.8: Dislocation spreading in a cubic grain at $\varepsilon_p = 10^{-3}$ in cases : (a) $N = 5 \times 10^{20} \text{m}^{-3}$ defects, D = 50 nm (the dispersed defects are not shown in this case, for clarity), (b) $N = 6 \times 10^{21} \text{m}^{-3}$ defects, D = 5 nm, (c) $N = 5 \times 10^{20} \text{m}^{-3}$ defects, D = 15 nm, (d) $N = 1.5 \times 10^{21} \text{m}^{-3}$ defects, D = 15 nm. (e) Solid symbols: actual internal stress evolution calculated in a 2D mesh ($800 \times 800 \text{ nm}^2$) comprising 72×72 discrete points, cutting through the y axis indicated in Fig. 4.8d. Dashed line: internal stress evolution according to Eq. (4.15), using $l = 1/2D_g = 0.5 \mu \text{m}$, $k_{\text{max}} = 1.75$ and $\tau_{app} = 138 \text{ MPa}$ (from Fig. 4.3a and Schmid factor 0.41). The τ_{int} magnitude (or τ_{int}/τ_{app} ratio) is nearly maximal in position (1).



FIGURE 4.9: Plastic strain spreading effect at different temperatures. (a) Stress-stain response. (b) Dislocation density versus plastic strain.

tance, the dislocation density at $\varepsilon_p = 10^{-3}$ with $T_0 = 350$ K is almost 2 times of the value achieved at $T_0 = 250$ K. It means that higher straining temperature induces faster dislocation multiplication rate, thus associated with increased dislocation activity. The present results are in good agreements with experimental observations (Kuramoto et al., 1979), DD (Chaussidon et al., 2010) and FEM (Singh et al., 2017) simulation results.

At each fixed straining temperature, we then introduce various defect dispersions into the grains, with a view to investigate the corresponding dislocation mobility evolutions, focusing on D = 15 nm loop size and defect number density $N = 1000 - 5000 \times 10^{18} \text{m}^{-3}$. The Δ DIAT evolutions obtained with different straining temperatures are shown in Fig. 4.10. At $T_0 = 250$ K, the Δ DIAT magnitude almost linearly increases with respect to the defect number density. In the other 2 cases, the Δ DIAT increases from $N = 1000 \times 10^{18} \text{m}^{-3}$ to $N = 3000 \times 10^{18} \text{m}^{-3}$ and then is saturates around 80 K and 90 K, respectively. For a fixed defect number density N, the Δ DIAT magnitude increases with the straining temperature, especially for $N > 1000 \times 10^{18} \text{m}^{-3}$.

Interestingly, the Δ DIAT evolutions with straining temperature closely reflect the corresponding fracture toughness response evolutions as shown in Fig. 4.11a. Namely the impact energy shift increases with the straining temperature ($T_0 > T'_0$). This evolution is consistent with enhanced multiplication and propagation of dislocation populations near the fracture surface of the tested specimens. This effect directly relates to rate of dislocation/defect interaction as evaluated during the DD simulations. In the $N = 3000 \times 10^{18} \text{m}^{-3}$ case for example, the dislocation/defect interaction count at $T_0 = 350 \text{K}$ is almost four times higher than at $T_0 = 250 \text{ K}$ (for a fixed $\varepsilon_p = 10^{-3}$). The (screw) dislocation population activity is then more pronounced at higher straining temperature, where the presence of defect dispersion has a larger relative impact, in terms of dislocation mobility, as shown in Fig. 4.11b. This situation explains that ($T_0 - T_1$) > ($T'_0 - T'_1$) for $T_0 > T'_0$ and hence, the DIAT shift increases with the straining temperature.

We have therefore shown that the influence of a given defect dispersion (characterized



FIGURE 4.10: Δ DIAT as functions of the defect number density *N*, for different straining temperatures.



FIGURE 4.11: Straining temperature effect. (a) Typical resilience curves obtained in unirradiated and irradiated materials, with $T_0 > T'_0$. (b) Screw dislocation velocity versus the effective resolved shear stress, for different straining temperatures. Subscript 0 represents the dislocation motion in unirradiated grain and subscript 1 indicates the irradiated case.

by N and D) on dislocation mobility increases with the straining temperature, as does the fracture toughness response evolutions. In the forthcoming section, we will alternatively discuses the grain size and grain orientation effects on the DIAT shift.

4.2 Grain size effect

The stress-strain responses of $1 \,\mu\text{m}$ and $2 \,\mu\text{m}$ defect-free grains are shown side by side, in Fig. 4.12a. The initial applied stress level (where $\varepsilon_p < 2 \times 10^{-4}$) is proportional to $1/\sqrt{D_g}$, i.e. consistent with the well-known Hall-Petch effect, associated with the internal stress landscape where the dislocations store at the grain boundaries. The workhardening rate is limited, in agreement with the stress-strain response of poly-crystalline BCC metals (Böhmert and Müller, 2002). The mean applied stress level is consistent with the observed mobile dislocation densities (see Fig. 4.12b), given the selected (controlled) plastic strain rate conditions and the adopted stress-velocity rules. The dislocation density accumulation rate is linear with the cumulated plastic strain, in both Grain 1 and Grain 2 cases. At a fixed plastic strain level, the dislocation density in Grain 2 is slightly lower than in Grain 1, despite the relatively large applied stress gap between the two cases. A comparable effect is observed in MD simulations (Hahn and Meyers, 2015) using similar boundary conditions as specified in Section 2. In the present DD simulations, the dislocation structures take the form of individual shear bands, whose number density increases with the rising strain level and disperse defect number density (Chaussidon et al., 2008; Robertson and Gururaj, 2011; Chaussidon et al., 2010). Dislocation multiplication inside individual shear bands is due to the formation dislocation sources (in the form of openloops) and very active cross-slip (Chaussidon et al., 2008; Louchet and Saka, 2003). In these conditions, it can be shown that the actual shear band thickness and spacing are consistent with the internal stress field evolutions (Gururaj et al., 2015a; Robertson et al., 2007). In any case, the observed grain size effect on the dislocation density accumulation rate is in good agreement with earlier DD simulation results and direct experimental evidence (Chaussidon et al., 2008; Gururaj et al., 2015b; Robertson et al., 2007; Robertson and Gururaj, 2011; Chaussidon et al., 2010).

The (average) applied stress level is dose-dependent (see Fig. 4.3a), i.e. increases with the defect number density (Böhmert and Müller, 2002). This effect mainly depend on the dislocation mobility rules and dislocation/facet interaction mechanisms that are likewise, grain-size independent.

The DIAT shift amplitude corresponding to each simulation case is then calculated using Eq. (4.12)-(4.13) and plotted in Fig. 4.13 below (solid symbols). For a fixed grain size, the DIAT shift increases with the defect size and number density, up to a specific, case-dependent saturation level. In Grain 2 and D = 25 nm case for example, the Δ DIAT level saturates at 95 K for a defect number density $N > 10^{21}$ m⁻³. For a fixed irradiation condition, larger grain size induces higher Δ DIAT, especially with small defect number density. In D = 25 nm case for instance, Δ DIAT increases from 38 K ($D_g = 1 \mu$ m) to 71 K ($D_g = 2 \mu$ m), at 5×10^{20} m⁻³ defect number density. According to Fig. 4.12, increasing the grain size (at fixed strain rate) induces lower applied stress and dislocation accumulation



FIGURE 4.12: Plastic strain spreading in defect-free Grain 1, Grain2 and Grain 3 simulation setups. (a) Stress-strain response. (b) Dislocation density evolution with cumulated plastic strain. Grain 1, Grain 2 and Grain 3 labels are defined in Tab. 4.2.

rate, which means dislocation propagations in larger grain become much easier yielding more mobile dislocations. Therefore the influence of defect dispersions in Grain 2 is relatively more important than that in Grain 1 in terms of statistical dislocation mobility, which finally results in a larger Δ DIAT amplitude. The grain size effect is significantly smaller for higher defect densities (see Fig. 4.13b), where the dislocation/defect interaction rate is dominant, in terms of dislocation multiplication mechanism.

4.3 Grain orientation effect

The grain orientation effect is evaluated by comparing the DD simulation results associated with Grain 2 and 3 setups (see Section 2.2.1). The applied stress and dislocation density evolutions with plastic strain in defect-free case are shown in Figs. 4.12a and 4.12b.

The significant grain orientation dependence hereby is due to decreased activity in the first slip system. In the second slip system however, the dislocation density is almost unchanged, for the two tested grain orientations. It is understood that these evolutions closely reflect the Schmid factors evolutions indicated in Tab. 4.3. Obtaining the exact form of the grain orientation-dependence on Δ DIAT involves further theoretical developments. In principle however, a grain orientation yielding a lower Schmid factor (in either the primary or cross-slip systems) is also associated with a smaller internal stress field and finer shear bands (see also Fig. 4.15 and Gururaj et al. (2015a)). This interpretation is validated by the simulation results to be presented in the next sections.

The grain-orientation effect on the Δ DIAT evolutions is presented in Fig. 4.14, showing a similar trend as in Fig. 4.13. The Δ DIAT level is systematically lower in the $z = (\bar{1}54)$ oriented Grain 3 than in the z = (100) oriented Grain 2, however. In the D = 25 nm cases, Δ DIAT achieves a saturation level for about $N = 10^{21} \text{m}^{-3}$ in Grain



FIGURE 4.13: Δ DIAT evolutions for different defect number densities, in Grain 1 and Grain 2 simulation setups. Grain size effect for different defect number density cases : (a) defect size D = 15 nm, (b) defect size D = 25 nm. Solid symbols : DD simulation results using Eq. (4.13); dashed lines : Eq. (4.14) prediction for corresponding D and N inputs. Adjustment of Δ DIAT data with analytical Eq. (4.14) is further discussed below, in Section 5.

2 and $N > 1.5 \times 10^{21} \text{m}^{-3}$ in Grain 3. It is interesting to note that for fixed defect size, the saturation level is mostly independent of the grain orientation. This situation especially applies to large defect number density cases, where the dislocation multiplication is dominated by the dislocation/defect interactions.

5 General discussions and $\Delta DIAT / \Delta DBTT$ correlation

All the Δ DIAT results presented in this work can be described (i.e. adjusted) using Eq. (4.14), including three independent scaling parameters. We found that ΔT_{max} and λ are grain-size and grain orientation independent, at least in the conditions of this study.

In practice, Fig. 4.13 data can be adjusted using Eq. (4.14) by varying the shear band thickness parameter, namely by using d = 320 nm with Grain 2 data and d = 220 nm with Grain 1 data (see Tab. 4.4). Similarly, Fig. 4.14 data can be adjusted using Eq. (4.14) with d = 280 nm for Grain 3 data and d = 320 nm for Grain 2 data (see also Tab. 4.4). The shear band thicknesses obtained by adjusting Δ DIAT data with Eq. (4.14) are in any case consistent with the simulation-generated dislocation microstructures (see Fig. 4.15 below). Thicker shear bands are found in larger grains (since $d \propto \sqrt{D_g}$) and generate a higher DIAT shift, for a given defect dispersion. Increasing the grain size indeed facilitates dislocation cross-slip, which is consistent with thicker shear bands and a more pronounced evolution of the dislocation mobility (with respect to the defect-free case). Changing the grain orientation significantly affect the Δ DIAT level, for a given grain size. This particular effect is associated with corresponding change in the applied resolved shear stress repartition, among the different slip systems. This effect most probably contributes to the



FIGURE 4.14: Δ DIAT evolutions using Grain 2 and Grain 3 simulation setups for various defect dispersion cases : grain orientation effect. Solid symbols : DD simulation results using Eq. (4.13); dashed lines : Eq. (4.14) prediction for corresponding *D* and *N* inputs. Adjustment of Δ DIAT data with Eq. (4.14) is further discussed below, in Section 5.

 Δ DIAT scattering, in poly-crystalline aggregates.

TABLE 4.4: Shear band thickness parameter *d* estimated by adjusting Eq. (4.14) on Δ DIAT simulation results. The data is consistent with $d \propto \sqrt{D_g}$. This means, for example, that $d(D_g = 10 \,\mu\text{m}) = d(D_g = 1 \,\mu\text{m}) \times \sqrt{10 \,\mu\text{m}/1 \,\mu\text{m}} = \sqrt{10} \times 220 \,\text{nm} \sim 700 \,\text{nm}$.

	Grain 1	Grain 2	Grain 3
Shear band thickness d	220 nm	320 nm	280 nm

The Δ DIAT levels reported in this work closely reflect the actual dose-dependent Δ DBTT data associated with irradiation conditions (and materials) compatible with the present study (Matijasevic et al., 2008, 2009; Baluc et al., 2007; Hishinuma et al., 1998; Nikolaev et al., 2002; Rieth et al., 1998, 2013; Nishiyama et al., 1998; Porollo et al., 1998; Ghoneim and Hammad, 1997; Kuleshova et al., 2002; Kocik et al., 2002; Jia and Dai, 2003). Fig. 4.16a presents the case of Fe-2.25%Cr VVER-1000 steel irradiated to different neutron doses, at two different temperatures. The Δ DBTT data set (1) corresponds to irradiation temperature $T_{irr} = 400$ °C, neutron dose range $10^{22} - 5 \times 10^{23} \text{m}^{-2}$ and grain size $D_g = 10 \,\mu\text{m}$ (shear band thickness $d \sim 700 \,\text{nm}$: see Tab. 4.4 caption) (Nishiyama et al., 1998). For a fixed irradiation temperature, the defect size is mostly dose-independent, while the defect number density linearly augments with the neutron dose (or fluence) (Matijasevic et al., 2008; Bruemmer et al., 1999). The defect size $D = 7 \,\text{nm}$



FIGURE 4.15: Dislocation structures at the same plastic strain level: grain size and grain orientation effects. The defects are not shown for clarity. (a) Grain 2, (b) Grain 3 simulation setups (see Tab. 4.2). The configuration of Grain 1 is shown in Fig. 4.8. The shear band thicknesses are consistent with the Δ DIAT based values calculated using Eq. (4.14) and reported in Tab. 4.4.

and number densities N corresponding to data set (1) are evaluated based on TEM observations (Porollo et al., 1998). Similarly, Δ DBTT data set (2) corresponds to irradiation temperature $T_{irr} = 288 \,^{\circ}$ C, neutron fluence range $7 \times 10^{23} - 1.4 \times 10^{24} \text{m}^{-2}$ and grain size $D_g = 2 \,\mu\text{m}$ (shear band thickness $d \sim 320 \,\text{nm}$) (Ghoneim and Hammad, 1997). The defect size $D = 5 \,\text{nm}$ and number densities N associated with data set (2) come from (Kuleshova et al., 2002; Kocik et al., 2002). The Δ DIAT curves A and B are calculated with Eq. (4.14) using D, d and N values associated with data sets (1) and (2), respectively; whereas $\Delta T_{\text{max}} = 110 \,^{\circ}$ C and $\lambda = 11 \,\text{nm}$ (see Section 3.3).

Interestingly, we found that Eq. (4.14) also applies to ferritic alloys of different Cr concentrations. Fig. 4.16b presents two different Fe-9%Cr steel cases, Eurofer97 and F82H, irradiated to different neutron doses, at 300 °C. The Δ DBTT data set ③ corresponds to Eurofer97 steel, neutron doses 0.3-2.5 dpa and lath (or grain) size $D_g = 1 \mu m$ (shear band thickness $d \sim 220 \text{ nm}$) (Matijasevic et al., 2008). The defect size D = 15 nm and number densities N associated with data set ③ are taken from (Matijasevic et al., 2008). The Δ DBTT data set ④ corresponds to F82H steel, neutron doses 0.2-2.5 dpa and lath (or grain) size $D_g = 2 \mu m$ (shear band thickness $d \sim 320 \text{ nm}$) (Rieth et al., 1998). The defect size D = 7 nm and defect densities N corresponding to data set ④ are taken from (Jia and Dai, 2003). The Δ DIAT curves C and D are calculated with Eq. (4.14) using D, d and N values associated with data sets ③ and ④, respectively (using $\Delta T_{\text{max}} = 110 \text{ °C}$ and $\lambda = 11 \text{ nm}$, as before).

The Δ DIAT versus Δ DBTT equivalence reported in Fig. 4.16 can be rationalized as follows. Brittle fracture in ferritic materials is governed by the cleavage initiator distributions (carbide particles, for example) (Forget et al., 2016). This situation can be statisti-



b)

FIGURE 4.16: Comparison between calculated Δ DIAT results and actual Δ DBTT data obtained for different ferritic materials and neutron irradiation conditions. (a) Case of Fe-2.25%Cr VVER-1000 steel irradiated to different neutron doses, at two different temperatures. Δ DBTT data sets ① and ② (solid symbols) are associated with Δ DIAT curves A and B (dashed lines), calculated using Eq. (4.14) with corresponding input data. (b) Case of two different Fe-9%Cr steels irradiated to different neutron doses at 300 °C: F82H and Eurofer97. Δ DBTT data sets ③ and ④ (solid symbols) are associated with Δ DIAT curves C and D (dashed line), calculated using Eq. (4.14) with the corresponding input data.

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cally treated using the weakest-link theory (Anderson et al., 1994), in combination with crystal plasticity modelling (Vincent et al., 2010; Libert et al., 2011). The fracture probability associated with a given dose level then only depends on the stress field acting on the cleavage initiators (see Eq. (7) in p. 300 of reference Besson et al. (2006)). This perception is consistent with the well-known empirical correlation $\Delta DBTT \sim \eta \Delta \sigma_{app}$ (Sokolov et al., 2004), where $\Delta \sigma_{app}$ is the irradiation-induced increase of the yield stress and η the proportionality factor (in K/MPa units). Likewise, we have seen that changing the grain size affects the dislocation sub-structure characteristic dimensions (see Fig. 4.15) and associated internal stress landscape τ_{int} . The corresponding $\Delta DIAT$ trends (cf. Figs. 4.13 and 4.14) indicate that the $\exp(-D/\lambda)$ and $\exp(-d^2DN)$ terms in Eq. (4.14) actually scale with sub-grain $\sigma_{int}/\sigma_{app}$ evolutions which finally makes it $\Delta DIAT \sim \theta \Delta \sigma_{app}$ (see Section 3.4 and Gururaj et al. (2015a)), where θ is expressed in K/MPa units. Factor $\eta \approx \theta$ in Fe-2.25%Cr grains and therefore $\Delta DIAT \approx \Delta DBTT$ for a broad σ_{app} domain, compatible with the materials and irradiation conditions as documented in Fig. 4.16.

The reader should keep in mind that the current Δ DIAT framework is exclusively based on dislocation-mediated plasticity mechanisms. This approach characterizes the brittle-ductile transition through the quantitative dislocation mobility changes associated with defect dispersion populations, regardless of the defect type (dislocation loop, vacancy loop, voids or others) involved. In certain irradiation conditions, additional physical causes may also contribute to the dose-dependent fracture response evolutions. For example, the $\Delta DBTT$ level is systematically higher in presence of significant segregating element concentrations at grain boundaries and/or particle/matrix interfaces (He for example (Rieth et al., 1998) and Chap. 6 in (Was, 2016)). This means segregations have a distinct contribution to the DBTT shift, adding up to the plasticity mechanisms considered in Section 2.3. It is therefore expected that $\Delta DBTT > \Delta DIAT$ under a certain (yet to be explored) range of irradiation conditions. Accounting for these effects entails further investigation effort, by means of adapted simulation methods (for example of the segregation effect: Yamaguchi (2011)). In its current form, Eq. (4.14) best applies to irradiation conditions where interfacial segregations, helium production, included particle dissolution or grain size changes are limited, i.e. for relatively low dose and irradiation temperature conditions in ferritic steels. The limiting radiation condition specified in this Section is at best indicative (dose < 2-3 dpa, irradiation temperature T_{irr} < 400 °C), being associated with the largest disperse defect size tested herein.

6 Conclusions

Plastic strain spreading in cubic Fe-Cr grains is investigated by means of 3D DD simulations. The effect of defect dispersions on dislocation motions is thereby examined, in controlled strain rate, tensile loading conditions, accounting for thermally activated slip and cross-slip, at room temperature. The main results are summarized below:

1. The defect-induced Δ DIAT evolutions are caused by corresponding dislocation mobility changes;

- 2. Both the straining temperature and the defect dispersions impact the effective dislocation mobility;
- 3. The specific Δ DIAT simulation trends herein can be explained in terms of a shear band model (e.g. Eqs. (4.14) and (4.15)). More specifically, the actual Δ DIAT dependence on the defect number density *N* and size *D* is characterized by three different material-dependent scaling parameters, namely: the reference temperature shift ΔT_{max} , the screw dislocation mean free path λ and the strain-induced shear band thickness *d*;
- 4. For a fixed irradiation condition, the Δ DIAT level increases with the straining temperature, in agreement with the corresponding resilience test results (Δ DBTT), due to exactly the same straining temperature evolution;
- 5. For a given defect dispersion, the Δ DIAT amplitude increases with the grain size, depending on the grain orientation;
- 6. The reported Δ DIAT evolutions scale with the shear band thickness parameter *d* that itself is grain size and grain orientation dependent;
- 7. The Δ DIAT level obtained for a disperse defect size *D* and defect number density *N* case closely reflect the experimentally-observed ductile to brittle transition temperature shift (Δ DBTT) associated with exactly the same, actual *D* and *N* case.

The Δ DIAT concept is developed with a view to facilitate the prediction of dosedependent DBT temperature shift evolutions, based on direct observation/measurement of the radiation-induced defect populations. More precisely, DBT shift evolutions can be estimated using Eq. (4.14) together with actual material microstructure (EBSD analysis, for example) and radiation-induced disperse defect (SANS measurements, for example) observation data. This approach can potentially help reducing the need for costly and timeconsuming post-irradiation mechanical testing in hot cells and provide valuable complementary information, especially if used in combination with conventional surveillance techniques.

Chapter 5

Conclusions and perspectives

Plastic deformation in irradiated materials involves mutual dislocation interactions and their interactions with defect clusters and impurities embedded in the matrix. Accurate modelling of these short-range (local) and long-range interactions is crucial for understanding material degradations taking place in the nuclear radiation environment. Three dimensional dislocation dynamics is a computational tool linking the small-scale and large-scale interaction mechanisms, characterizing microstructural evolutions across vastly different length and time scales. This thesis employed the DD formalism, for examining the following three issues:

- 1. Study the migration and the interactions of prismatic dislocation loops in α -iron;
- 2. Study the role of the cross-slip in the scene of dislocation/defect interactions;
- 3. Study the statistic evolution of dislocation mobility in ferritic grains populated with radiation-induced defects.

Features	Chapter 2	Chapter 3	Chapter 4
Materials	α–iron		Ferritic steel
Defects	$\langle 111 \rangle$ -prismatic loops		$\langle 100 \rangle$ -facet dispersions
Scales	Isolated dislocation and/or prismatic loop		Grain
Loadings	Thermal fluctuations	Peicewise stress	Strain rate
DD Techniques	Node-based		Screw-Edge based
Software	NUMODIS		TRIDIS
Discretization Length	\sim Å		\sim nm
Time Step	\sim fs		\sim ns

TABLE 5.1: DD simulation features of each chapter in this thesis.

The simulation details of each chapter are summarized in Tab. 5.1. It is visible that more than half of this manuscript deals with elementary dislocation behaviours, using node-based DD technique (NUMODIS code). In Chapter 2, the diffusion of individual prismatic dislocation loop and interacting loop-pairs has been simulated using the same

DD framework accounting for the stochastic forces associated with the thermal fluctuations. Owing to its accurate description of the dislocation topology, both internal and collective dynamics of prismatic loops have been successfully captured, highlighting on the loop tilting effect. In Chapter 3, the cross-slip effect on dislocation/loop interactions is investigated using the same DD code. In this case, a specific composite dislocation source setup associated with a cross-slipped dislocation segment has been developed and implemented. That approach allowed the evaluation of the separate contribution of the loop-induced stress field on the dislocation by-passing mechanism, by replacing the loop with a hard facet.

The rest of the manuscript (Chapter 4) focuses on the examination of dislocation evolutions acting at the grain scale, using segment-based DD simulations (TRISDIS code) accounting for the thermally activated dislocation slip and cross-slip mechanisms. Implementation of the loop-facet setup allows calculating the strain spreading and evolution of the dislocation microstructure in ferritic grains in presence of dispersed defects. The defect-induced evolutions of the effective screw dislocation mobility are then evaluated using Defect-Induced Apparent Straining Temperature shift (Δ DIAT) concept.

The most significant results presented in this manuscript are:

- 1. The study of single prismatic loop diffusion has shown that the temperaturedependence of the diffusion coefficient is consistent with both molecular dynamics simulation results and the fluctuation-dissipation theorem.
- 2. The loop-pair simulation cases have revealed that the internal degrees of freedom generate complex potential energy landscape states depending on the loop habit plane orientations. The energy contribution associated with the thermal fluctuations enables interacting loops to switch between the various tilted configurations, that helps overcoming the potential energy barrier.
- 3. Comparison with various theoretical solutions (pure prismatic loops) have shown that the interacting loop reorientation can strongly affect the elastic confinement of loops. Firstly, loop reorientation can significantly reduce the potential barrier for the elastic trapping. Secondly, loop reorientation can result in a dramatic increase in the elastically confined state lifetime.
- 4. The isolated dislocation/loop interaction simulations have shown that the presence of a cross-slipped segment can greatly facilitate dislocation source unpinning from a defect, thus reducing its effective obstacle strength. Moreover, it is shown that the composite dislocation source response only depends on the force acting on the dislocation section connecting the segments gliding in different slip planes, regardless of the particular loop interaction mechanism and stress field.
- 5. Cross-slip thus appears to be the dominant strain rate limiting mechanism during dislocation-mediated straining in presence of radiation-generated defect dispersions.
- 6. The facet-loop surrogate approach can significantly improve the computational efficiency without the loss in the accuracy when characterizing the dislocation mobility in presence of the cross-slip.

- 7. The simplified dislocation/facet descriptions, thermally activated mobility rules and cross-slip algorithm employed in massive DD simulations are capable to reproduce the plastic deformation observed in post-irradiated ferritic grains. The resulting dislocation microstructure and the plastic response are consistent with the experimental observations.
- 8. For a given defect dispersion (size and number density), the effective mobility change of screw dislocations is characterized by a given Δ DIAT level. The Δ DIAT simulation trends can be explained in terms of plasticity mechanisms associated with shear band development. The obtained results qualitatively and quantitatively replicate the actual Δ DBTT evolutions due to the corresponding defect dispersion evolutions.
- The noted ADIAT/ADBTT correlation can be interpreted based on plastic strain spreading arguments. The brittle to ductile transition temperature are then possibly controlled by defect-induced changes of the effective dislocation mobility.

The thesis work takes advantage of both node-based and segment-based DD simulations, which present distinct pros and cons. The main difference lies on dislocation topology associated with distinct discretization methods. The node-based DD simulations allow a precise and accurate description on the evolution of the dislocation microstructure. Node-based simulation are therefore powerful in studying local dislocation behaviours with fine discretization length, e.g. the internal dynamics of dislocation loop and the individual dislocation/defect interactions. However, the time step size is typically limited by the response of the most unstable dislocation node. These gains thus comes at the cost of small time steps.

On the other hand, the segment-based DD simulations discretize dislocations into predefined segments (e.g. screw-edge). Accordingly, the computational load associated with the dislocation-dislocation interaction, which is the most time-consuming step in DD frameworks, could be significantly reduced. This type of DD method is thus beneficial for characterizing the ensemble behaviour of dislocation populations at relatively large length and time scales (see Tab. 5.1 for example).

The above listed results draw the following perspectives:

- 1. The time step used in Chapter 2 is very small, which prevents the direct use of our model at a larger scale. Incidentally, the viscous drag coefficient based on experimental data is much higher than that calibrated from the molecular dynamics results. In principle, the use of experimentally observed drag coefficients allows extending time steps up to three order of magnitude larger.
- 2. The step by step calculation of the elastic interactions bears a high computational cost. The implementation of acceleration method is therefore highly desirable. Such methods include parallelization, fast dislocation-induced stress calculation schemes (fast multiple method) and simplified viscous drag matrix calculations.
- 3. The current stochastic DD framework can be applied to analyze several poorly understood mechanisms. For example, dislocations act as the sink for radiation

defects and their reactions with prismatic loops also entail in long-range elastic interactions. It is thus expected that loop reorientation may affect these interactions as well. Moreover, the study of loop migration and growth/shrinkage can be undertaken by incorporating proper dislocation climb rules.

- 4. The implementations of cross-slip and kink-pair mechanism in DD simulations can be revisited/improved for both BCC and FCC structures, with the aid of the molecular dynamics simulations.
- 5. The systematic study of effective screw dislocation mobility in irradiated materials can be further explored, using more advanced theoretical models. The grain size and grain orientation effects on $\Delta DIAT/\Delta DBTT$ can help analyzing the defect dispersion effect in polycrystalline materials.
- 6. Radiation dose accumulation can cause a reduction in the upper shelf energy (USE) of Charpy impact curves. It is believed that this effect is intimately related with the flow localization and the corresponding loss of ductility, as shown various times in this manuscript (see Chapter 1 for example). The quantitative analysis of USE decrease and strain localisation mechanisms entails further effort to be pursued in the next future.

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